

REPORT DOCUMENTATION PAGE			Form Approved OMB NO. 0704-0188		
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1. REPORT DATE (DD-MM-YYYY) 18-08-2010		2. REPORT TYPE Final Report		3. DATES COVERED (From - To) 1-Oct-2009 - 30-Jun-2010	
4. TITLE AND SUBTITLE Ordered Rate Constitutive Theories: Development of Rate Constitutive Equations for Solids, Liquids, and Gases			5a. CONTRACT NUMBER W911NF-09-1-0548		
			5b. GRANT NUMBER		
			5c. PROGRAM ELEMENT NUMBER 611102		
6. AUTHORS Karan S. Surana, J. N. Reddy, Albert Romkes			5d. PROJECT NUMBER		
			5e. TASK NUMBER		
			5f. WORK UNIT NUMBER		
7. PERFORMING ORGANIZATION NAMES AND ADDRESSES University of Kansas Center for Research, Inc. 2385 Irving Hill Road  Lawrence, KS 66045 -7563			8. PERFORMING ORGANIZATION REPORT NUMBER		
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) U.S. Army Research Office P.O. Box 12211 Research Triangle Park, NC 27709-2211			10. SPONSOR/MONITOR'S ACRONYM(S) ARO		
			11. SPONSOR/MONITOR'S REPORT NUMBER(S) 57395-MA-II.1		
12. DISTRIBUTION AVAILABILITY STATEMENT Approved for Public Release; Distribution Unlimited					
13. SUPPLEMENTARY NOTES The views, opinions and/or findings contained in this report are those of the author(s) and should not be construed as an official Department of the Army position, policy or decision, unless so designated by other documentation.					
14. ABSTRACT In this research, the rate constitutive theories for ordered thermoviscous fluids, ordered thermoelastic solids and ordered thermoviscoelastic polymeric fluids in contra- and co-variant bases are developed. Such theories are necessitated when the mathematical models of the deforming matter are derived using the Eulerian description. In each case, the dependent variables in the rate constitutive theory and their argument tensors describing the physics of the deforming matter are identified. The dependent variables in the constitutive theory are expressed as a linear					
15. SUBJECT TERMS Rate Constitutive Theories, Solids, Fluids, Polymers					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT UU	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON Karan Surana
a. REPORT UU	b. ABSTRACT UU	c. THIS PAGE UU			19b. TELEPHONE NUMBER 785-864-2988

## Report Title

Ordered Rate Constitutive Theories: Development of Rate Constitutive Equations for Solids, Liquids, and Gases

### ABSTRACT

In this research, the rate constitutive theories for ordered thermoviscous fluids, ordered thermoelastic solids and ordered thermoviscoelastic polymeric fluids in contra- and co-variant bases are developed. Such theories are necessitated when the mathematical models of the deforming matter are derived using the Eulerian description. In each case, the dependent variables in the rate constitutive theory and their argument tensors describing the physics of the deforming matter are identified. The dependent variables in the constitutive theory are expressed as a linear combination of the combined generators of the argument tensors. The coefficients in the linear combinations are functions of the combined invariants of the argument tensors, temperature, and density (for compressible matter; in the current configuration). The coefficients in the linear combination are determined by considering their Taylor's series expansions about the reference configuration and limiting the expansion to linear terms in the combined invariants and temperature.

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### List of papers submitted or published that acknowledge ARO support during this reporting period. List the papers, including journal references, in the following categories:

#### (a) Papers published in peer-reviewed journals (N/A for none)

Karan S. Surana, Yongting Ma, Albert Romkes, and J. N. Reddy, The Rate Constitutive Equations and their Validity for Progressively Increasing Deformation, Journal of Mechanics of Advanced Materials and Structures, In Press, 2010.

Karan S. Surana, Daniel S. Nunez, J. N. Reddy, and Albert Romkes, Rate Constitutive Theory for Ordered Thermofluids, In Process of Being Submitted.

Karan S. Surana, Daniel S. Nunez, J. N. Reddy, and Albert Romkes, Rate Constitutive Theory for Ordered Thermoelastic Solids, in Process of Being Submitted.

Karan S. Surana, Daniel S. Nunez, J. N. Reddy, and Albert Romkes, Rate Constitutive Theory for Ordered Thermoviscoelastic Fluids - Polymers, in Process of Being Submitted.

Number of Papers published in peer-reviewed journals: 4.00

---

#### (b) Papers published in non-peer-reviewed journals or in conference proceedings (N/A for none)

Number of Papers published in non peer-reviewed journals: 0.00

---

#### (c) Presentations

Number of Presentations: 0.00

---

#### Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts): 0

---

#### Peer-Reviewed Conference Proceeding publications (other than abstracts):

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts): 0

---

#### (d) Manuscripts

Karan S. Surana, Daniel S. Nunez, J. N. Reddy, and Albert Romkes, Rate Constitutive Theory for Ordered Thermo fluids, In Process of Being Submitted.

Karan S. Surana, Daniel S. Nunez, J. N. Reddy, and Albert Romkes, Rate Constitutive Theory for Ordered Thermoelastic Solids, in Process of Being Submitted.

Karan S. Surana, Daniel S. Nunez, J. N. Reddy, and Albert Romkes, Rate Constitutive Theory for Ordered Thermoviscoelastic Fluids - Polymers, in Process of Being Submitted.

Number of Manuscripts: 3.00

Patents Submitted

Patents Awarded

Graduate Students

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
Daniel S. Nunez	0.50
Yong-Ting Ma	0.50
Tristan Moody	0.50
FTE Equivalent:	1.50
Total Number:	3

Names of Post Doctorates

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>	National Academy Member
Karan S. Surana	0.09	No
J. N. Reddy	0.03	No
FTE Equivalent:	0.12	
Total Number:	2	

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### Student Metrics

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Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:..... 0.00

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### Names of Personnel receiving masters degrees

NAME

Total Number:

### Names of personnel receiving PhDs

NAME

Total Number:

### Names of other research staff

NAME

PERCENT SUPPORTED

FTE Equivalent:

Total Number:

### Sub Contractors (DD882)

1 a. Texas Engineering Experiment Station

1 b. Research Services

Texas Engineering Experiment Station

College Station TX 778454645

**Sub Contractor Numbers (c):** FY2010-033

**Patent Clause Number (d-1):**

**Patent Date (d-2):**

**Work Description (e):**

**Sub Contract Award Date (f-1):** 10/1/2009 12:00:00AM

**Sub Contract Est Completion Date(f-2):** 6/30/2010 12:00:00AM

---

1 a. Texas Engineering Experiment Station

1 b. Office of Sponsored Research

3000 TAMU

College Station TX 778433000

**Sub Contractor Numbers (c):** FY2010-033

**Patent Clause Number (d-1):**

**Patent Date (d-2):**

**Work Description (e):**

**Sub Contract Award Date (f-1):** 10/1/2009 12:00:00AM

**Sub Contract Est Completion Date(f-2):** 6/30/2010 12:00:00AM

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**Inventions (DD882)**

# **Ordered Rate Constitutive Theories**

## **Report**

**Prepared under STIR Grant Proposal:**

### **Development of Rate Constitutive Equations for Solids, Liquids and Gases**

by

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**Final Report Submitted to**

**Army Research Office**

Attn: Dr. Joseph D. Myers  
Mathematical Sciences Division  
U.S. Army Research Office  
P.O. Box 12211

Research Triangle Park, NC 27709-2211  
Under the STIR Grant number: W911NF-09-1-0548(FED0065623)

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# Chapter 1

## Continuum Mechanics Principles and Axioms of Constitutive Theory, and Scope of the Present Research

### 1 Introduction

The development of the mathematical models for deforming matter using conservation laws [1, 2] is independent of the constitution of the matter. The stress field and heat vector are assumed to be a consequence of kinematics of deformation in the deforming matter without regard to the specific nature of the matter. However, we know that same disturbance applied to different matters will undoubtedly produce different response. It is obvious that the mathematical models from the conservation laws do not have a closure. This is rightfully so, due to the fact that without matter-specific details the mathematical models from the conservation laws are unable to describe behaviors of the deforming matter.

For simple solids and fluids, the relationships between the stress field and deformation and between heat vector and temperature gradients are referred to as the constitutive equations. Development of these relations is the subject matter of study in the constitutive theory. For a deforming matter to be in thermodynamic equilibrium, conservation laws must be satisfied. The conservation of mass, application of Newton's second law to a volume of deforming matter, and the first law of thermodynamics yield continuity equation, momentum equations and the energy equation, respectively. An additional condition or law essential for thermodynamic equilibrium is the second law of thermodynamics, namely, the Clausius-Duhem inequality, commonly referred to as the entropy inequality. Thus, for thermodynamic equilibrium to exist in deforming matter in addition to three basic conservation law, the entropy inequality must also be satisfied.

How should we proceed in the development of the constitutive theory that establishes the stress field and heat vector (and others) in terms of the physics of deforming matter and its properties? We could view the development of the constitutive equation in the following three ways:

- (i) Since the three basic conservation laws only require existence of the stress field and heat vector, the development of the constitutive equations is not the focus in these laws and hence they provide no mechanism for deriving the constitutive theory. However, we must ensure these conservation laws are not violated in the development of the constitutive theory. Thus, the second law of thermodynamics or entropy inequality alone must provide a mechanism to derive the constitutive theory. In this approach entropy inequality is naturally satisfied by the constitutive theory as it is derived from it. In this process we may also utilize other conservation laws if so desired. This approach is appealing due to the fact that the constitutive theory resulting from this approach will naturally satisfy all conditions essential for thermodynamic equilibrium of the deforming matter.
- (ii) The second approach is based on the theory of generators and invariants and minimal basis. We express the stress tensor and heat vector as a linear combinations of the combined generators of the arguments

tensors. The coefficients in the linear combinations are assumed to functions of the combined invariants of the argument to functions of the combined invariants of the argument tensors and scalars. The coefficients are determined by expanding these in Taylor series about the reference configuration. This approach has continuum mechanics foundation but may be viewed to lack thermodynamic basis from the point of view that the derivations are not based on the second law of thermodynamics but the constitutive theory so derived can be made to satisfy the requirements resulting from the entropy inequality.

- (iii) In the third approach, we could derive constitutive equations independent of the entropy inequality as well as independent of the other principles and axioms of continuum mechanics but by using other means (such as empirical relations based on experimental evidence). However, we must show that the constitutive equations so derived indeed satisfy the Clausius-Duhem inequality otherwise the deformation process of the matter utilizing these constitutive equations in conjunction with GDEs from the three basic conservation laws will not be in thermodynamic equilibrium. Constitutive equations for power law fluids are examples of this approach.

It is obvious that the first approach, if plausible, is highly meritorious. Derivation of constitutive relation using Clausius-Duhem inequality is referred to as thermodynamic approach of deriving constitutive equations as this approach naturally ensures existence of thermodynamic equilibrium in the deforming matter. In the subsequent chapter we only consider approaches (i) and (ii) to derive the rate constitutive theory for incompressible as well as compressible solid matter and fluids.

It is well known that for deforming solid matter, Lagrangian descriptions are preferable. These descriptions provide the ability to monitor motion of material particles during the deformation process. The development of the constitutive theory for stress in Lagrangian description for solid matter using Green's strain (and others), second Piola-Kirchhoff stress etc. for deforming matter under finite deformation is relatively well established [1–3] and can be derived by using conditions resulting from the entropy inequality. Likewise the constitutive theory for the heat vector can also be established using the conditions resulting from the entropy inequality. This results in the well known Fourier heat conduction law.

When the mathematical models for deforming matter are derived using Eulerian description, then the material particle displacements and strain measures are not readily obtainable. In such mathematical models, velocities are the dependent variables of choice (as opposed to displacements in Lagrangian description). Thus, development of the constitutive theory in Eulerian description must consider a suitable coordinate system in the deformed configuration in which time derivatives of the chosen stress and strain tensors can be related. The constitutive theory so derived uses rates of stress and strain tensors in a convenient coordinate system and hence the name 'rate constitutive theory'. The same holds for the heat vector as well. Thus the first and the foremost decision is regarding a suitable coordinate system. If we consider homogeneous and isotropic matter and if we mark the orthogonal material lines in the reference configuration then upon deformation these result in curvilinear maps in the current configuration. The tangent vectors to these curvilinear material lines forming a non-orthogonal basis called co-variant basis are one of the natural choice for deriving the constitutive theory. Another possibility is to consider another non-orthogonal basis that is reciprocal to the co-variant basis. This is referred to as contra-variant basis. Thus, contra- and co-variant bases in the deformed configuration and the convected time derivatives of the chosen stress and strain measures in these bases must form the fundamental approach for deriving the rate constitutive theory in Eulerian description.

Another significant aspect of the constitutive theory is the decision on the choice of dependent variables in the constitutive theory and the argument tensors on which they depend. A specific form of constitutive equations define an ideal material. In the selection of the variables used in deriving constitutive equations certain physical and mathematical requirements must be satisfied. Thus in the development of the constitutive theory we intend to describe a limited physical phenomenon decided at the onset of the derivation. Even though there seems to be a lack of systematic mechanism to decide on the basic variables needed in the development of the constitutive equations, there are guiding axioms and principles that may be used to at least rule out certain variables from consideration in the development of the constitutive theory. The material presented in the following section is due to reference [2] but it is sufficiently condensed and focused to provide only a high level conceptual understanding of the basic axioms that must be followed in the development of the constitutive theory.

## 2 Axioms or principles of constitutive theory

The following axioms and principles are fundamental in the development of the constitutive theory [1, 2]: axiom of casualty, axiom of determinism, axiom of equipresence, axiom of objectivity, axiom of material invariance, axiom of neighborhood, axiom of memory, axiom of admissibility.

### (i) *Axiom of casualty*

Based on this principle we consider motion of the material points of a body and their temperatures as self-evident observable effect in every thermomechanical behavior of matter. The remaining quantities, other than those that can be derived using motion and temperature of material points that enter the expression of entropy generation or production are the ‘causes’ or dependent variables in the development of the constitutive theory.

As an example, in case of thermomechanical behavior of deforming matter, based on this principle, the independent variables are

$$\bar{\mathbf{x}} = \bar{\mathbf{x}}(\mathbf{x}, t), \quad \theta = \theta(\mathbf{x}, t) \quad (2.1)$$

Now the velocity can be derived using time derivatives of  $\bar{\mathbf{x}}$ , density in the current configuration is deterministic from the conservation of mass or continuity equation. Thus in describing the entropy production the quantities that remain to be prescribed are stress tensor  $\bar{\boldsymbol{\sigma}}$ , heat vector  $\bar{\mathbf{q}}$ , internal energy density  $e$  and entropy density  $\eta$ . These constitute dependent variables and hence must be expressed in terms of  $\bar{\mathbf{x}} = \bar{\mathbf{x}}(\mathbf{x}, t)$  and  $\theta = \theta(\mathbf{x}, t)$ .

### (ii) *Axiom of determinism*

The values of the thermomechanical function,  $(\bar{\boldsymbol{\sigma}}, \bar{\mathbf{q}}, e, \eta)$ , at a material point  $\mathbf{x}$  in the current configuration at time  $t$  is determined by the history of motion and temperature of all material points. Thus for material points  $\mathbf{x}'$  at time  $t' \leq t$  we have

$$\bar{\boldsymbol{\sigma}}(\mathbf{x}, t) = \bar{\boldsymbol{\sigma}}(\mathbf{x}(\mathbf{x}', t'), \theta(\mathbf{x}', t'), \mathbf{x}, t) \quad (2.2)$$

$$\bar{\mathbf{q}}(\mathbf{x}, t) = \bar{\mathbf{q}}(\mathbf{x}(\mathbf{x}', t'), \theta(\mathbf{x}', t'), \mathbf{x}, t) \quad (2.3)$$

$$e(\mathbf{x}, t) = e(\mathbf{x}(\mathbf{x}', t'), \theta(\mathbf{x}', t'), \mathbf{x}, t) \quad (2.4)$$

$$\eta(\mathbf{x}, t) = \eta(\mathbf{x}(\mathbf{x}', t'), \theta(\mathbf{x}', t'), \mathbf{x}, t) \quad (2.5)$$

We note that  $\mathbf{x}'$  and  $t'$  are functions of  $\mathbf{x}$  and  $t$ .

### (iii) *Axiom of equipresence*

At the onset of establishing all constitutive functionals these all must be expressed in terms of the same list of independent constitutive variables until the contrary is deduced. Thus we see the presence of  $\mathbf{x}(\mathbf{x}', t)$ ,  $\theta(\mathbf{x}', t)$ ,  $\mathbf{x}$  and  $t$  in all constitutive equations 2.2 - 2.5.

### (iv) *Principle of objectivity*

The constitutive equations must be form invariant with respect to rigid motion of the spatial frame of reference.

### (v) *Axiom of material invariance*

If the constitutive equations do not change when  $(x_1, x_2, x_3)$  are changed to  $(x_1, x_2, -x_3)$ , then this represents reflection of the material frame of reference with respect to the plane  $x_3 = 0$ . This may be due to crystallographic orientations of the material points in the matter. Thus according to this principle the constitutive equations must be form invariant under a group of orthogonal transformations representing planes of symmetry in the matter.

### (vi) *Axiom of neighborhood*

The values of the independent constitutive variables at distant material points from  $\mathbf{x}$  do not affect appreciably the values of the constitutive dependent variables at  $\mathbf{x}$ .

#### *Smooth neighborhood*

If the constitutive functionals are sufficiently smooth, they can be approximated by the functionals in the field of real functions. Based on this principle, Taylor’s series expansions hold in a neighborhood of a material

point  $\mathbf{x}$ .

**(vii) Axiom of memory**

The values of the constitutive variables at a distant past from the current configuration do not affect appreciably the values of the constitutive functions in the current configuration. This leads to the principles of smooth memory and fading memory (discussed later).

**(viii) Axiom of admissibility**

All constitutive equations must be consistent with the principles of continuum mechanics, i.e., the constitutive equations must satisfy conservation of mass, balance of momenta, conservation of energy and the second law of thermodynamics, i.e., entropy inequality or Clausius-Duhem inequality.

### 3 Second law of thermodynamics: Clausius-Duhem inequality or entropy inequality

The fundamental principles of continuum mechanics are conservation of mass, balance of momenta and conservation of energy leading to continuity, momentum and energy equations. These are well known in both Lagrangian and Eulerian descriptions and hence are not repeated here. In addition to these, for all deforming matter to be in thermodynamic equilibrium, the second law of thermodynamics, i.e., entropy inequality or Clausius-Duhem inequality must be satisfied. We discuss details of entropy inequality as it plays a central and crucial role in the development of the constitutive theory. Some of these details are intentionally repeated in the following chapter for the sake of clarity and completeness of presentation.

From thermodynamics point of view, entropy inequality is a statement of irreversibility in most natural processes especially those involving dissipation of energy, i.e., say conservation of mechanical energy into heat. From the point of view of continuum mechanics, Clausius-Duhem inequality contain much more information than just statement of irreversibility. Analogous to the assumption of contact forces, body forces in the application of Newton's second law to a deforming volume of matter and assumption of the heat fluxes, source of energy in the first law of thermodynamics, we can also postulate a similar statement for entropy. Consider a volume  $V$  of matter with closed boundary  $\partial V$  in the reference configuration. Upon deformation,  $V$  occupies  $\bar{V}(t)$  and  $\partial V$  occupies  $\partial\bar{V}(t)$  in the current configuration at time  $t$ .

Consider volume  $\bar{V}(t)$ . Let  $\bar{h}$  be the entropy flux between  $\bar{V}(t)$  and the volume of the matter surrounding it,  $\bar{s}$  be the source of entropy in  $\bar{V}(t)$  due to non-contacting bodies (considered per unit mass). Let there exist,  $\bar{\eta}$  the specific entropy (entropy per unit mass) for  $\bar{V}(t)$  bounded by  $\partial\bar{V}(t)$  such that its rate of increase is at least equal to that supplied to  $\bar{V}(t)$  from all source (containing or non-contacting). Thus

$$\frac{D}{Dt} \int_{\bar{V}(t)} \bar{\eta} \bar{\rho} d\bar{V} \geq \int_{\partial\bar{V}(t)} \bar{h} d\bar{s} + \int_{\bar{V}(t)} \bar{s} \bar{\rho} d\bar{V} \quad (3.1)$$

We adopt Cauchy's postulate for entropy flux  $\bar{h}$ , i.e.,  $\bar{h}$  at a point  $\bar{x}_i$  on  $\partial\bar{V}(t)$  depends upon the orientation  $\bar{n}$  of  $\partial\bar{V}(t)$  at  $\bar{x}_i$ . Hence we have

$$\bar{h} = -\bar{\Psi} \cdot \bar{n} \quad (3.2)$$

in which  $\bar{\Psi}$  is similar to heat flux. Substituting 3.2 into 3.1 gives

$$\frac{D}{Dt} \int_{\bar{V}(t)} \bar{\eta} \bar{\rho} d\bar{V} \geq - \int_{\partial\bar{V}(t)} \bar{\Psi} \cdot \bar{n} d\bar{s} + \int_{\bar{V}(t)} \bar{s} \bar{\rho} d\bar{V} \quad (3.3)$$

Using divergence theorem for the first term on the right side of 3.3 yields

$$\frac{D}{Dt} \int_{\bar{V}(t)} \bar{\eta} \bar{\rho} d\bar{V} \geq - \int_{\bar{V}(t)} \bar{\Psi}_{i,i} d\bar{V} + \int_{\bar{V}(t)} \bar{s} \bar{\rho} d\bar{V} \quad (3.4)$$

Consider the term on the left side of inequality in 3.4 and use  $\bar{\rho} d\bar{V} = \rho dV$  (conservation of mass). Hence

$$\frac{D}{Dt} \int_{\bar{V}(t)} \bar{\eta} \bar{\rho} d\bar{V} = \frac{D}{Dt} \int_V \eta \rho dV = \int_V \frac{D}{Dt} (\eta \rho) dV \quad (3.5)$$

but

$$\frac{D}{Dt} (\eta \rho) = \eta \frac{D\rho}{Dt} + \rho \frac{D\eta}{Dt} = \rho \frac{D\eta}{Dt} \quad (3.6)$$

as  $\frac{D\rho}{Dt} = 0$ . Substituting from 3.6 into 3.5 gives

$$\frac{D}{Dt} \int_{\bar{V}(t)} \bar{\eta} \bar{\rho} d\bar{V} = \int_V \rho \frac{D\eta}{Dt} dV = \int_V \frac{D\eta}{Dt} \rho dV = \int_{\bar{V}(t)} \bar{\rho} \frac{D\bar{\eta}}{Dt} d\bar{V} \quad (3.7)$$

By substituting from 3.7 into 3.4 we obtain

$$\int_{\bar{V}(t)} \bar{\rho} \frac{D\bar{\eta}}{Dt} d\bar{V} \geq - \int_{\bar{V}(t)} \Psi_{i,i} d\bar{V} + \int_{\bar{V}(t)} \bar{s} \bar{\rho} d\bar{V} \quad (3.8)$$

or

$$\int_{\bar{V}(t)} \left( \bar{\rho} \frac{D\bar{\eta}}{Dt} + \Psi_{i,i} - \bar{s} \bar{\rho} \right) d\bar{V} \geq 0 \quad (3.9)$$

Since  $\bar{V}(t)$  is arbitrary, we have

$$\bar{\rho} \frac{D\bar{\eta}}{Dt} + \Psi_{i,i} - \bar{s} \bar{\rho} \geq 0 \quad (3.10)$$

Equation 3.10 is the most general form of the entropy inequality also known as Clausius-Duhem inequality. In continuum mechanics a different form of (3.10) is often more meaningful as well as useful. If we assume that

$$\Psi = \frac{\bar{\mathbf{q}}}{\bar{\theta}} \quad , \quad \bar{s} = \frac{\bar{r}}{\bar{\theta}} \quad (3.11)$$

where  $\bar{\theta}$  is absolute temperature assumed to be greater than zero,  $\bar{\mathbf{q}}$  is heat vector and  $\bar{r}$  is a suitable potential. Using 3.11 gives

$$\Psi_{i,i} = \frac{\bar{q}_{i,i}}{\bar{\theta}} - \frac{\bar{q}_i}{(\bar{\theta})^2} \bar{\theta}_{,i} \quad (3.12)$$

Substituting from 3.12 into 3.10 yields

$$\bar{\rho} \frac{D\bar{\eta}}{Dt} + \left( \frac{\bar{q}_{i,i}}{\bar{\theta}} - \frac{\bar{q}_i}{(\bar{\theta})^2} \bar{\theta}_{,i} \right) - \frac{\bar{\rho} \bar{r}}{\bar{\theta}} \geq 0 \quad (3.13)$$

If we multiply through out by  $\bar{\theta}$  (as  $\bar{\theta} > 0$ ) then

$$\bar{\rho} \bar{\theta} \frac{D\bar{\eta}}{Dt} + (\bar{q}_{i,i} - \bar{\rho} \bar{r}) - \frac{\bar{q}_i \bar{\theta}_{,i}}{\bar{\theta}} \geq 0 \quad (3.14)$$

Expression 3.14 is the most common form of Clausius-Duhem inequality. 3.14 can be further given a different form using energy equation. Recall the energy equation in Eulerian description ( $\bar{\sigma}_{ij}^{(0)}$  contra-variant Cauchy stress tensor)

$$\bar{\rho} \frac{D\bar{e}}{Dt} + (\bar{\nabla} \cdot \bar{\mathbf{q}} - \bar{\rho} \bar{r}) - \bar{\sigma}_{ij}^{(0)} \frac{\partial v_i}{\partial \bar{x}_j} = 0 \quad (3.15)$$

$$\therefore \quad \bar{\nabla} \cdot \bar{\mathbf{q}} - \bar{\rho} \bar{r} = \bar{q}_{i,i} - \bar{\rho} \bar{r} = -\bar{\rho} \frac{D\bar{e}}{Dt} + \bar{\sigma}_{ij}^{(0)} \frac{\partial v_i}{\partial \bar{x}_j} \quad (3.16)$$

Substituting from 3.16 into 3.14

$$\bar{\rho}\bar{\theta}\frac{D\bar{\eta}}{Dt} - \bar{\rho}\frac{D\bar{e}}{Dt} + \bar{\sigma}_{ij}^{(0)}\frac{\partial v_i}{\partial \bar{x}_j} - \frac{\bar{q}_i\bar{\theta}_{,i}}{\bar{\theta}} \geq 0 \quad (3.17)$$

or

$$\bar{\rho}(\bar{\theta}\frac{D\bar{\eta}}{Dt} - \frac{D\bar{e}}{Dt}) + \bar{\sigma}_{ij}^{(0)}\frac{\partial v_i}{\partial \bar{x}_j} - \frac{\bar{q}_i\bar{\theta}_{,i}}{\bar{\theta}} \geq 0 \quad (3.18)$$

or

$$\bar{\rho}(\frac{D\bar{e}}{Dt} - \bar{\theta}\frac{D\bar{\eta}}{Dt}) - \bar{\sigma}_{ij}^{(0)}\frac{\partial v_i}{\partial \bar{x}_j} + \frac{\bar{q}_i\bar{\theta}_{,i}}{\bar{\theta}} \leq 0 \quad (3.19)$$

Let  $\Phi$  be the Helmholtz free energy density (specific Helmholtz free energy) defined by

$$\bar{\Phi} = \bar{e} - \bar{\eta}\bar{\theta} \quad (3.20)$$

$$\therefore \frac{D\bar{\Phi}}{Dt} = \frac{D\bar{e}}{Dt} - \bar{\eta}\frac{D\bar{\theta}}{Dt} - \bar{\theta}\frac{D\bar{\eta}}{Dt} \quad (3.21)$$

Hence

$$\frac{D\bar{e}}{Dt} - \bar{\theta}\frac{D\bar{\eta}}{Dt} = \frac{D\bar{\Phi}}{Dt} + \bar{\eta}\frac{D\bar{\theta}}{Dt} \quad (3.22)$$

Substituting from 3.22 into 3.19

$$\bar{\rho}(\frac{D\bar{\Phi}}{Dt} + \bar{\eta}\frac{D\bar{\theta}}{Dt}) + \frac{\bar{q}_i\bar{\theta}_{,i}}{\bar{\theta}} - \bar{\sigma}_{ij}^{(0)}\frac{\partial v_i}{\partial \bar{x}_j} \leq 0 \quad (3.23)$$

This is known as reduced form of Clausius-Duhem inequality in Eulerian or spatial description of motion. 3.23 plays important role in the development of the constitutive theory.

*Clausius-Duhem inequality in Lagrangian or material description:*

In this section we derive a form of 3.23 using Lagrangian description. In Lagrangian description, all quantities of interest are expressed as a function of  $x_i$ , coordinates of the material points in the reference configuration and time. We consider each term in 3.23

$$\rho = |J|\bar{\rho} \quad ; \quad [J] = \begin{bmatrix} \bar{x}_1, \bar{x}_2, \bar{x}_3 \\ x_1, x_2, x_3 \end{bmatrix} \quad (3.24)$$

$$\begin{aligned} \bar{q}_i(\bar{x}_i, t) &\rightarrow q_i(x_i, t) \\ \bar{\theta}_i(\bar{x}_i, t) &\rightarrow \theta_i(x_i, t) \end{aligned} \quad (3.25)$$

$$\begin{aligned} \{\bar{q}\} &= [J^t]^{-1}\{q\} \\ \{\bar{\nabla}\bar{\theta}\} &= [J^t]^{-1}\{\nabla\theta\} \end{aligned} \quad (3.26)$$

$$\bar{q}_i\bar{\theta}_{,i} = \{\bar{q}\}^t\{\bar{\nabla}\bar{\theta}\} \quad (3.27)$$

or

$$\bar{q}_i\bar{\theta}_{,i} = \{q\}^t([J]^{-1}[J^t]^{-1})\{\nabla\theta\} \quad (3.28)$$

Cartesian components of  $[\bar{\sigma}^{(0)}]$ , i.e.,  $[\sigma^{[0]}]$  and  $[\bar{\sigma}^{(0)}]$  are related through

$$[\bar{\sigma}^{(0)}] = |J|^{-1}[J][\sigma^{[0]}][J]^t \quad (3.29)$$

Also recall that

$$[L] = v_{i,j} \quad , \quad [\dot{J}] = [L][J] \quad (3.30)$$

$[\sigma^{[0]}]$  is of course second Piola-Kirchhoff stress and

$$\bar{\sigma}_{ij}^{(0)}v_{i,j} = \text{tr}([\bar{\sigma}^{(0)}][L]^t) = \text{tr}([\bar{\sigma}^{(0)}]^t[L]^t) \quad (3.31)$$

Substituting for  $[\bar{\sigma}^{(0)}]$  from 3.29 into 3.31

$$\bar{\sigma}_{ij}^{(0)} v_{i,j} = \text{tr}(|J|^{-1}[J][\sigma^{[0]}][J]^t[L]^t) = |J|^{-1} \text{tr}([J][\sigma^{[0]}][\dot{J}]^t) \quad (3.32)$$

Substituting from 3.24 - 3.32 into 3.23

$$\rho|J|^{-1} \left( \frac{D\Phi}{Dt} + \eta \frac{D\theta}{Dt} \right) + \frac{\{q\}^t ([J]^{-1} [J^t]^{-1}) \{\nabla \theta\}}{\theta} - |J|^{-1} \text{tr}([J][\sigma^{[0]}][\dot{J}]^t) \leq 0 \quad (3.33)$$

Since  $\Phi = \Phi(x_i, t)$  and  $\theta = \theta(x_i, t)$  then

$$\frac{D\Phi}{Dt} = \frac{\partial \Phi}{\partial t} \quad ; \quad \frac{D\theta}{Dt} = \frac{\partial \theta}{\partial t} \quad (3.34)$$

Substituting from (3.34) into (3.33) and multiplying through out by  $|J|$ , we obtain

$$\rho \left( \frac{\partial \Phi}{\partial t} + \eta \frac{\partial \theta}{\partial t} \right) + \frac{|J| \{q\}^t ([J]^{-1} [J^t]^{-1}) \{\nabla \theta\}}{\theta} - \text{tr}([J][\sigma^{[0]}][\dot{J}]^t) \leq 0 \quad (3.35)$$

Equation 3.35 is the entropy inequality in Lagrangian description or material description of motion.

## 4 Preliminary considerations in the development of the constitutive theory

From the entropy inequality we note it contains stress  $\bar{\sigma}_{ij}^{(0)}$ , heat vector  $\bar{q}_i$ , specific internal energy  $\bar{e}$  and entropy density  $\bar{\eta}$  in Eulerian description and  $\sigma_{ij}^{[0]}$ ,  $q_i$ ,  $e$  and  $\eta$  in Lagrangian description. The choice of  $\bar{e}$ ,  $\bar{\eta}$  or  $\bar{\Phi}$ ,  $\bar{\eta}$  is a matter of preference as they are related through  $\bar{\Phi}$ . Likewise the choice of  $e$ ,  $\eta$  or  $\Phi$ ,  $\eta$  is a matter of preference also as these are also related through  $\Phi$ . We consider  $\bar{\Phi}$ ,  $\bar{\eta}$  and  $\Phi$ ,  $\eta$  in the details that follow. In the work presented here we only consider homogeneous and isotropic matter in which all points consist of the same material particles. Thus for homogeneous and isotropic matter, the constitutive theory at a point are valid for the entire volume of matter. We consider two classifications of the matter.

### *Materials without memory:*

In such materials the path taken to arrive at the present configuration is invariant. That is for such materials the current configuration has no memory of how it is arrived at. Such material clearly have no concept of relaxation. Newtonian fluids, generalized Newtonian fluids, elastic solids are examples of material without memory.

### *Materials with memory:*

Viscoelastic solids, polymeric liquids on the other hand are examples of materials with memory. For such materials, the path to arrive at the current configuration is important. Such materials have concept of relaxation, i.e., when the disturbance is removed the material continue to relax relieving stresses and eventually reaches the relaxed state. For such materials there is a time constant called relaxation time that characterizes their relaxation behavior. In the work presented here we consider materials without memory as well as those with memory.

### *Choice of variables in constitutive theory and methodology*

For simple materials such as elastic solids, thermoelastic solids, thermoviscoelastic solids, Newtonian fluids, polymers etc. the objective of the constitutive theory is to provide a mathematical foundation for quantitatively establishing the stress field and heat vector in the deforming matter as a functions of tensors that are measures of the deforming matter's physics in the current configuration. Thus stress tensor and heat vector are undoubtedly the dependent variables in the constitutive theory. Also, entropy inequality derivation suggests that we have a choice between Helmholtz free energy density  $\Phi$  or ( $\bar{\Phi}$ ) and entropy density  $\eta$  or  $\bar{\eta}$ . We choose Helmholtz free energy  $\Phi$  or ( $\bar{\Phi}$ ) as the third dependent variable in the development of the constitutive theory.

Thus at the onset, one choice of dependent variables in the constitutive theory are  $\sigma, q, \Phi$  (or  $\bar{\sigma}, \bar{q}, \bar{\Phi}$ ).  $\sigma, q, \Phi$  are functions of argument tensors describing the physics of the deforming matter. At the onset we consider

principle or axiom of equipresence and consider all possible tensors as arguments of  $\sigma$ ,  $q$ ,  $\Phi$ . Some of these may be ruled out at a later stage due to other considerations. Amongst all of the axiom of constitutive theory, the axiom of equipresence (used above), axiom of objectivity (form invariance) and the axiom of admissibility are most important in the development of the constitutive theory.

For a specific matter under consideration, once the argument tensors for  $\sigma$ ,  $q$ ,  $\Phi$  are determined that are in agreement with the axioms of the constitutive theory, we proceed as follows.

#### **Approach (1)**

Due to axiom of admissibility, all constitutive equations must satisfy conservation laws. Conservation of mass, balance of momenta and conservation of energy are independent of the constitution of the matter. Their derivation assume existence of the stress field and heat vector. Thus, what remains in the second law of thermodynamics or Clausius-Duhem inequality. That is, all constitutive equations must satisfy entropy inequality. Said differently, if we use entropy inequality to derive constitutive equations then it will naturally be satisfied by the resulting theory. In continuum mechanics this is the fundamental approach for deriving constitutive equations. Using this approach it is possible:

- (a) To derive constitutive equations for the heat vector for all matters (within some assumptions).
- (b) For elastic and thermoelastic solid matter, the stress field in a deforming matter can be established in terms of the chosen strain measure in the Lagrangian description.
- (c) Additionally, thermodynamic and mechanical pressure (Stoke hypothesis) can also be established as part of the constitutive theory.
- (d) For matters other than solids in which Eulerian description is necessary to derive mathematical models, the entropy inequality only provides mechanism for establishing mechanical and thermodynamic pressures with the additional restriction that energy dissipation due to the deviatoric stress be positive, but provides no explicit mechanism for establishing the constitutive theory.

#### **Approach (2)**

In deforming matter in which entropy inequality does not provide an explicit mechanism for deriving constitutive theory, i.e., for solids and fluids (both incompressible and compressible) for which mathematical models utilize Eulerian description, we use an alternate approach. By examining the constitutive equations for elastic solid matter and thermoelastic solid matter in Lagrangian description derived using entropy inequality, we note that the expression for the stress tensor is a linear combination of the combined generators [1, 2] of the argument tensors. This observation suggests an approach for deriving constitutive equations in which the stress tensor is expressed as a linear combination of the combined generators of the argument tensors. The coefficients in the linear combination are functions of the combined invariants of the argument tensors (and other quantities) and are determined using their Taylor's series expansions about the reference configuration (as in approach (1)). In this approach we do have to ensure that energy conversion due to the deviatoric stress is positive, a requirement from the entropy inequality.

#### **Remarks:**

The two approach listed above ((1) and (2)) provide a unified theory. We do remark that approach (1) is strictly in accordance with entropy inequality and hence has thermodynamic basis and is well established in the Lagrangian framework. Whereas, approach (2) has continuum mechanics foundation in the sense that it utilizes continuum mechanics axioms and principles and can be made to satisfy the condition of positive dissipation due to the deviatoric stress, a requirement resulting from the entropy inequality. However, in this approach, the constitutive theory is not derivable directly from the second law of thermodynamics.

## 5 Scope of the present research

### 5.1 Background

In this research, the rate constitutive theories for ordered thermoviscous fluids, ordered thermoelastic solids and ordered thermoviscoelastic polymeric fluids in contra- and co-variant bases are developed. Such theories are necessitated when the mathematical models of the deforming matter are derived using the Eulerian description. In each case, the dependent variables in the rate constitutive theory and their argument tensors describing the physics of the deforming matter are identified. The dependent variables in the constitutive theory are expressed as a linear combination of the combined generators of the argument tensors. The coefficients in the linear combinations are functions of the combined invariants of the argument tensors, temperature  $\bar{\theta}$ , and density  $\bar{\rho}$  (for compressible matter), where  $\bar{\theta}$  and  $\bar{\rho}$  are in the current configuration. The coefficients in the linear combination are determined by considering their Taylor's series expansions about the reference configuration and limiting the expansion to linear terms in the combined invariants and temperature  $\bar{\theta}$ .

As shown in section 4, the dependent variables in the rate constitutive theory must be the stress tensor, heat vector and Helmholtz free energy density. The stress tensor and heat vector must be considered in either contra- or co-variant basis. It is shown that in the development of the rate constitutive theories, the second law of thermodynamics, i.e., Clausius-Duhem inequality, does not provide any mechanism for the derivation of the constitutive theory for the total stress tensor. This is resolved by decomposing the total stress tensor in equilibrium stress and deviatoric stress. For compressible matter (solid or fluid) the conditions resulting from the entropy inequality establish equilibrium stress as the thermodynamic pressure that is a function of  $\bar{\theta}$  and  $\bar{\rho}$ . In the case of incompressible matter, the Clausius-Duhem inequality in conjunction with incompressibility constraint establish the equilibrium stress as the mechanical pressure which is a function of  $\bar{\theta}$ . Hence, the constitutive equations for the equilibrium stress are completely determined for compressible as well as incompressible thermoelastic solids as well as thermofluids and thermoviscoelastic fluids. In short, the rate constitutive theory must consider the deviatoric stress tensor, heat vector, and Helmholtz free energy density as dependent variables in contra- and co-variant bases. Details of each of the three general rate constitutive theories and their simplifications, essential in obtaining currently used constitutive equations, are considered in this work and are outlined in the following. In all cases we only consider homogeneous and isotropic matter.

### 5.2 Rate constitutive theory for ordered thermofluids

The rate constitutive theory for ordered thermofluids is presented in Chapter 2. The deviatoric stress tensor, heat vector, and Helmholtz free energy density are dependent variables in this constitutive theory. It is shown that for this type of matter, Helmholtz free energy density  $\bar{\Phi}$  is a function of  $\bar{\rho}$  and  $\bar{\theta}$  for compressible matter. For incompressible matter,  $\bar{\Phi}$  only depends on  $\bar{\theta}$ . The argument tensors for the deviatoric stress and heat vector are  $\bar{\rho}$ ,  $\bar{\theta}$ , temperature gradient  $\bar{\mathbf{g}}$ , and convected time derivatives of up to order ' $n$ ' of the chosen strain measure (Green's strain tensor in co-variant basis and Almansi strain tensor in the contra-variant basis) that are fundamental kinematic quantities. The combined generators and invariants of the argument tensors are used in the development of the rate constitutive theory. Derivations are presented in co-variant and contra-variant bases for both incompressible as well as compressible cases. It is shown that the constitutive equations for Newtonian fluids and generalized Newtonian fluids are rate constitutive equations and are special cases of ordered thermofluids of order one.

### 5.3 Rate constitutive theory for ordered thermoelastic solids

The rate constitutive theory for ordered thermoelastic solids is presented in Chapter 3 in co-variant and contra-variant bases. The density, temperature and temperature gradient in the current configuration and the convected time derivatives of the strain tensor (in a chosen basis) up to order ' $n$ ' are considered as argument tensors of the first convected time derivative of the deviatoric stress and heat vector in the chosen basis. The Helmholtz free energy density is a function of  $\bar{\rho}$  and  $\bar{\theta}$  or just  $\bar{\theta}$ , depending upon whether the matter is compressible or incompressible. The general theory derived using combined generators and invariants of the argument tensors is specialized for thermoelastic solids of order one and further simplified to show that commonly used constitutive theory for hypo-elastic solids is in fact a subset of the rate theory of order one.

## 5.4 Rate constitutive theory for ordered thermoviscoelastic fluids

The development of the rate constitutive theory for compressible as well as incompressible polymeric fluids is presented in Chapter 4. The polymeric fluids are considered as ordered thermoviscoelastic fluids in which the deviatoric stress rate of a desired order, i.e., the convected time derivative of a desired order ' $m$ ' of the chosen deviatoric stress tensor, and the heat vector are functions of density, temperature, temperature gradient, convected time derivatives of the chosen strain tensor up to any desired order ' $n$ ' and the convected time derivative of up to orders ' $m - 1$ ' of the chosen deviatoric stress tensor. The development of the constitutive theory is presented in both contra-variant as well as co-variant bases. The polymeric fluids described by this constitutive theory will be referred to as ordered thermoviscoelastic fluids due to the fact that the constitutive equations are dependent on the orders ' $m$ ' and ' $n$ ' of the convected time derivatives of the deviatoric stress and strain tensors. The highest orders of the convected time derivative of the deviatoric stress and strain tensors define the orders of the polymeric fluid. General rate theory of constitutive equations for ordered thermoviscoelastic fluids is also specialized to obtain commonly used constitutive equations for Maxwell, Giesekus, and Oldroyd-B constitutive models in contra- and co-variant bases.

## 5.5 Validity of co-variant and contra-variant rate constitutive theory for progressively increasing deformation

The research presented herein evaluates the validity of the rate constitutive theories in contra- and co-variant bases for progressively increasing deformation. The co-variant and contra-variant convected bases in the current configuration of the deforming matter provide two possible alternatives of defining convected time derivatives of the contra- and co-variant Cauchy stress tensors and the strain tensors. Relationship between the convected time derivatives of the stress tensor, material tensor and convected time derivative of the strain tensor result in the rate constitutive equations. Thus there are at least two obvious approaches for deriving rate constitutive equations: one based on co-variant description referred to as lower convected rate constitutive equations and the other based on contra-variant description referred to as upper convected rate constitutive equations. It can be shown that the other rate constitutive equations available in the literature can also be derived using these descriptions by making modifications that are either justified based on the physics of the deforming matter or mathematical manipulations. When the strains and the strain rates are small (closer to infinitesimal assumption), there is isomorphism (or equivalence) between the co-variant and contra-variant descriptions; hence, in this case the two descriptions will yield identical results even though the explicit forms of the rate equation expressions in the two descriptions are different. It is shown that when the strains and the strain rates are finite, the isomorphism or equivalence between the two descriptions is lost. This work demonstrates that with progressively increasing deformation leading to finite deformation only the contra-variant description has physical basis and, therefore, the rate constitutive theory derived using contra-variant description remain valid whereas all others become spurious. Numerical examples are also presented using Giesekus constitutive model for dense polymeric liquids (polymer melts) to demonstrate the validity of contra-variant basis and the failures of co-variant and others commonly used in the literature.

## 5.6 Summary, conclusions, and future work

Chapters 2 through 4 contain summaries and conclusions related to the work presented in each chapter. Overall summary of the work, its relevance in developing mathematical models for various matters under varied deformations, its importance in terms of a general and unified theory for all matter whose mathematical models are derived in the Eulerian description, and the potential of the general theory to enable more realistic and mathematically rigorous constitutive models are discussed in Chapter 6. It is shown that most constitutive models in the Eulerian description can be derived from the general rate theories presented in this research. Limitation of the theories developed herein and future research work in the constitutive theory are also discussed in Chapter 6.

## References:

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## Chapter 2

# Rate Constitutive Theory for Ordered Thermofluids

In this chapter we consider developments of constitutive theory for compressible as well as incompressible ordered homogeneous and isotropic thermofluids in which the deviatoric Cauchy stress tensor and the heat vector are functions of density, temperature, temperature gradient and the convected time derivatives of the strain tensors of up to a desired order. The developments of the constitutive theory are presented in both contra- and co-variant bases. The fluids described by these constitutive equations are known as ordered thermofluids due to the fact that the constitutive equations for the deviatoric Cauchy stress tensor and heat vector are dependent on the convected time derivatives of the strain tensor up to a desired order, the highest order of the convected time derivative of the strain tensor in the argument tensors defines the ‘order of the fluid’.

The admissibility requirement necessitates that the constitutive theory for the stress tensor and heat vector satisfy conservation laws, hence, in addition to conservation of mass, balance of momenta, and conservation of energy, the second law of thermodynamics, i.e., Clausius-Duhem inequality must also be satisfied by the constitutive equations or be used in their derivations. If we decompose the total Cauchy stress tensor into equilibrium and deviatoric components, then Clausius-Duhem inequality and Helmholtz free energy density can be used to determine the equilibrium stress in terms of thermodynamic pressure for compressible fluids and in terms of mechanical pressure for incompressible fluids with the additional requirement that the viscous dissipation due to the deviatoric Cauchy stress be positive, but the second law of thermodynamics provides no mechanism for deriving the constitutive theory for the deviatoric Cauchy stress tensor.

In the development of the constitutive theory one must consider a coordinate system in the current configuration in which the deformed material lines can be identified. Thus the co-variant and contra-variant convected coordinate systems are natural choices for the development of the constitutive theory. Furthermore, the mathematical models for fluids require Eulerian description with velocities as dependent variables. This precludes the use of displacement gradients, i.e., strain measures, in the development of the constitutive equations for such matter. It is shown that compatible conjugate pairs of convected time derivatives of the deviatoric Cauchy stress and strain measures in co- and contra-variant bases in conjunction with the theory of generators and invariants provide a general mathematical framework for the development of constitutive theory for ordered thermofluids. This framework has a foundation based on the basic principles and axioms of continuum mechanics and satisfies the condition of positive viscous dissipation, a requirement resulting from the entropy inequality. We present a general theory of constitutive equations for ordered thermofluids which is then specialized, assuming first order thermofluids, to obtain the commonly used constitutive equations for incompressible and compressible Newtonian, generalized Newtonian and other fluids. It is demonstrated that the constitutive theory for ordered thermofluids of all orders is indeed rate constitutive theory.

The research work presented in this chapter is being submitted for journal publication [1].

# 1 Introduction

Broadly speaking, all fluids can be classified into two categories: fluids without memory and those with memory. A fluid without memory has no recollection of how the current configuration is arrived at. For such fluids the only correspondence of the current configuration is to the reference configuration. On the other hand, fluids with memory have recollection of past events. If the recollection is limited to immediately preceding few events then we say that the fluid has fading memory. Fluids with memory naturally exhibit relaxation phenomenon. Such fluids upon cessation of the disturbance require finite amount of time to resume to a relaxed (unstressed) state dependent on the characteristic constant of the fluid, called relaxation time. Incompressible and compressible Newtonian fluids, generalized Newtonian fluids and many other fluids described by higher order theories involving the symmetric part of the velocity gradient tensor are examples of fluids without memory. Dilute polymeric liquids generally described by Maxwell model and Oldroyd-B model, and dense polymeric liquids described by Giesekus model, PTT model etc. are examples of fluids with memory. In the work presented here we only consider the development of the constitutive theory for fluids without memory.

Newton's law of viscosity for incompressible fluids and its extension for compressible medium are well known and widely used as constitutive equations for incompressible and compressible thermoviscous fluids (Newtonian fluids) [2, 3]. The constitutive models for generalized Newtonian fluids, such as power law and Carreau-Yasuda model, are extensions of the constitutive models for Newtonian fluids in which the medium viscosity is assumed to depend on the deformation field [4]. In fluid mechanics and gas dynamics books, both undergraduate and graduate level as well as monographs on fluid mechanics and gas dynamics, the importance of the constitutive models is emphasized from the point of view that we should know what they are, how to use them and do they predict what is observed experimentally. The emphasis on the mathematical details and the principles of continuum mechanics used (if any) in their derivations are virtually nonexistent in these writings. On the other end of the spectrum, the developments in continuum mechanics in the last three decades have been overwhelming [5–8]. These have been largely initiated and focused on solid matter with applications to liquids and gases (Newtonian fluids). While the basic definitions and the measures such as kinematics of deformation, measures of stresses, strains, their rates etc. do not distinguish between the specific nature of the matter and hence are equally applicable to solids, liquids and gases, this is not the case in the development of the constitutive theory due to the obvious fact that the constitutive equations are mathematical descriptions that are specific for a given type of matter. Thus the developments in the constitutive theory for solid matter can be useful when considering liquids and gases but these can not be imported in their entirety and used for liquids and gases. This is primarily due to the fact that the composition and behavior of liquids and gases are drastically different than solids, hence completely new considerations may be necessary in the development of the constitutive theory for such matter compared to those for solid matter.

The first account of ordered fluids seems to have appeared in reference [4] in connection with 'retarded motion expansion' defined as a deviation from Newtonian fluids. It was advocated that retarded motion expansion is the correct constitutive equation for flows in which rate-of-strain tensor and its time derivatives are small. The works in reference [9–12] are the basis for the presentations of ordered fluids in reference [4]. In these works, the stress tensor is considered as a polynomial in the convected time derivatives of progressively increasing orders of the strain rate tensors. While in simplified cases this may yield the same results as presented in the present work, in general, we observe three fundamental problems in these works: (i) Lack of derivation based on the second law of thermodynamics which necessitates decomposition of the Cauchy stress tensor into equilibrium stress and deviatoric stress. While the equilibrium stress is deterministic from the Clausius-Duhem inequality, the deviatoric stress is not. For the deviatoric stress one must use the theory of generators and invariants as opposed to the polynomial approach [4, 9–12]. (ii) In case of thermofluids, the constitutive theory must also address the constitutive equation for the heat vector. (iii) Co- and contra-variant bases and the development of the constitutive theory in these two bases and the differences in the resulting constitutive equations are not addressed.

We intentionally do not take an issue of the fact that whether these fluids have memory or elasticity. This aspect is briefly mentioned in reference [4]. In a subsequent chapter on 'rate constitutive theory for ordered thermoviscoelastic fluids - polymers' this aspect is discussed in detail. Here we present a general constitutive theory for the stress tensor and heat vector for ordered thermofluids using the second law of thermodynamics and the theory of generators and invariants. The general theory is also simplified to obtain the constitutive equations for the well known generalized Newtonian and Newtonian fluids. The developments of the constitu-

tive theory are presented using co- and contra-variant bases for incompressible as well as compressible cases. The consequences of the choice of basis are discussed and illustrated in the general derivation as well as for specialized cases.

## 2 Coordinate system, bases, measures of stresses and strains and their convected time derivatives

### 2.1 Co-variant and contra-variant bases

Consider undeformed matter in the reference configuration at time  $t_0$  (could be assumed zero) shown in figure 2.1(a). The reference configuration is assumed to be the same as the configuration of the matter at time  $t_0$ . Consider a volume of matter  $V$  with closed boundary  $\partial V$  and an elementary tetrahedron  $oABC$  with its face  $ABC$  coincident with the boundary  $\partial V$ . Let  $ox_1x_2x_3$  be an orthogonal Cartesian coordinate system located at point  $o$  (in the matter or outside the matter). Then each material particle can be assigned a unique label  $(x_1, x_2, x_3)$ , its coordinates being in  $ox_1x_2x_3$  frame, and hence uniquely identified. Assume that the matter is homogeneous and isotropic. Let  $ox_1, ox_2, ox_3$  parallel to  $x_1, x_2, x_3$  axes of the  $ox_1x_2x_3$  frame be the material lines coincident and co-linear with the edges of the tetrahedron  $oABC$  (figure 2.1(a) and (b)).

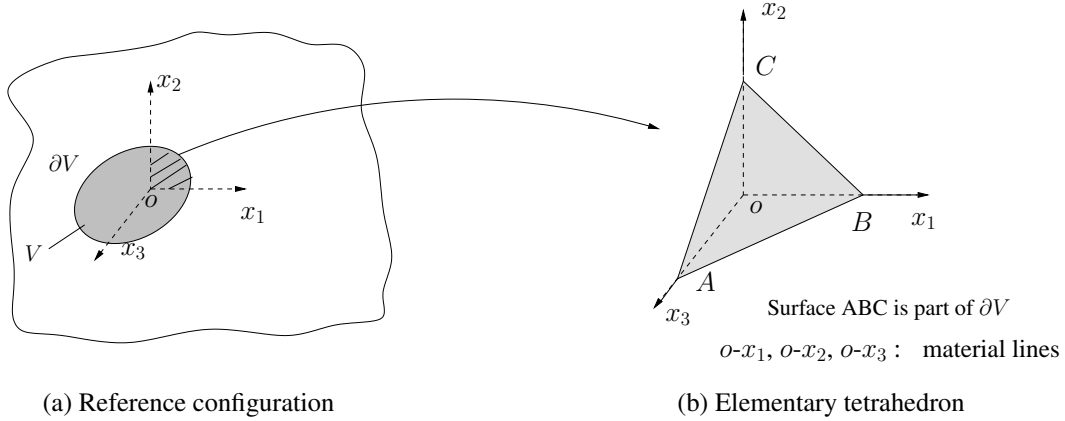


Figure 2.1: Elementary tetrahedron in the reference configuration

Upon deformation the material particles assume position in the current configuration (figure 2.2) at time  $t$ . The volume  $V$  deforms into  $\bar{V}(t)$  with its boundary  $\partial\bar{V}(t)$ . The elementary tetrahedron  $oABC$  deforms into  $\tilde{o}\tilde{A}\tilde{B}\tilde{C}$  with its deformed edges  $\tilde{o}\tilde{A}$ ,  $\tilde{o}\tilde{B}$  and  $\tilde{o}\tilde{C}$  tangent to the curvilinear axes  $\tilde{o}\tilde{x}_1$ ,  $\tilde{o}\tilde{x}_2$  and  $\tilde{o}\tilde{x}_3$ . The coordinate system  $\tilde{o}\tilde{x}_1\tilde{x}_2\tilde{x}_3$  is called convected coordinate system. If  $\bar{P}$  is the resultant force exerted on the face  $\tilde{A}\tilde{B}\tilde{C}$  of the deformed tetrahedron with volume of matter surrounded by boundary  $\partial\bar{V}(t)$  and if  $\bar{n}$  is the unit exterior normal to the face  $\tilde{A}\tilde{B}\tilde{C}$  of the deformed tetrahedron, then by considering equilibrium of the deformed tetrahedron we could develop various measures of stresses acting on the deformed faces  $\tilde{o}\tilde{A}\tilde{B}$ ,  $\tilde{o}\tilde{B}\tilde{C}$  and  $\tilde{o}\tilde{C}\tilde{A}$  of the tetrahedron  $\tilde{o}\tilde{A}\tilde{B}\tilde{C}$ . Likewise, conjugate strain measures can be derived as well. The convected coordinate system  $\tilde{o}\tilde{x}_1\tilde{x}_2\tilde{x}_3$  is crucial in developing constitutive equations due to the fact that this coordinate system defines deformed material lines in the current configuration.

Let the vectors  $\tilde{g}_1$ ,  $\tilde{g}_2$  and  $\tilde{g}_3$  be tangent to the  $\tilde{o}\tilde{x}_1$ ,  $\tilde{o}\tilde{x}_2$  and  $\tilde{o}\tilde{x}_3$  at material point  $\tilde{o}$ . The vectors  $\tilde{g}_i$  (not normalized) are called the co-variant vectors, which define a non-orthogonal basis and form the faces of the deformed tetrahedron. We can also introduce another set of base vectors called reciprocal base vectors  $\tilde{g}^i$  using

$$\tilde{g}^1 = (\tilde{g}_2 \times \tilde{g}_3) \quad ; \quad \tilde{g}^2 = (\tilde{g}_3 \times \tilde{g}_1) \quad ; \quad \tilde{g}^3 = (\tilde{g}_1 \times \tilde{g}_2) \quad (2.1)$$

where the base vectors  $\tilde{g}^i$  are called contra-variant base vectors. We note that  $\tilde{g}^1$  is normal to the face  $\tilde{o}\tilde{A}\tilde{C}$  formed by the co-variant base vectors  $\tilde{g}_2$  and  $\tilde{g}_3$ . Likewise  $\tilde{g}^2$  and  $\tilde{g}^3$  are normal to the faces  $\tilde{o}\tilde{A}\tilde{B}$  and  $\tilde{o}\tilde{B}\tilde{C}$

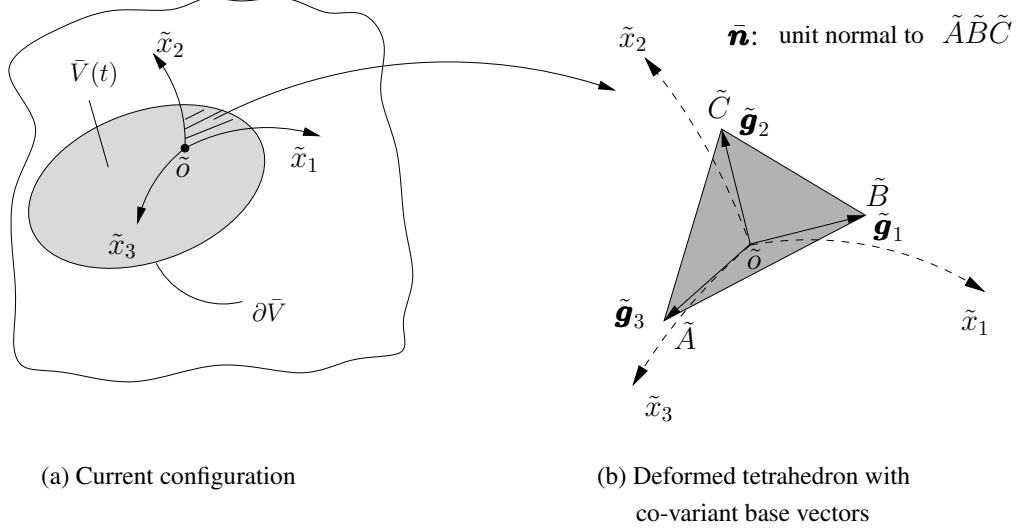


Figure 2.2: Deformed elementary tetrahedron in the current configuration

of the deformed tetrahedron  $\tilde{o}\tilde{A}\tilde{B}\tilde{C}$ . The volume of the deformed parallelepiped formed by the vectors  $\tilde{\mathbf{g}}_i$  is given by  $\tilde{V} = \tilde{\mathbf{g}}_1 \cdot (\tilde{\mathbf{g}}_2 \times \tilde{\mathbf{g}}_3)$ . Using 2.1 it is straight forward to see that the following holds:

$$\tilde{\mathbf{g}}^i \cdot \tilde{\mathbf{g}}_j = \tilde{\mathbf{g}}_i \cdot \tilde{\mathbf{g}}^j = \tilde{V} \delta_{ij} \quad (2.2)$$

where  $\delta_{ij}$  is Kronecker delta.

If we designate the coordinates of the material points in the current configuration by  $\bar{x}_1, \bar{x}_2, \bar{x}_3$ , measured with respect to  $ox_1x_2x_3$  frame, then a material point in the current configuration can be identified by

$$\bar{x}_i = \bar{x}_i(x_1, x_2, x_3, t) \quad (2.3)$$

Inverse of 2.3 is given by

$$x_i = x_i(\bar{x}_1, \bar{x}_2, \bar{x}_3, t) \quad (2.4)$$

If  $\{dx\} = [dx_1, dx_2, dx_3]^t$  and  $\{d\bar{x}\} = [d\bar{x}_1, d\bar{x}_2, d\bar{x}_3]^t$  are the components of length  $ds$  and  $d\bar{s}$  in the reference and current configuration, and if we neglect the infinitesimals of orders two and higher in both configurations, then we can obtain the following [13]:

$$\{d\bar{x}\} = [J]\{dx\} \quad (2.5)$$

$$\{dx\} = [\bar{J}]\{d\bar{x}\} \quad (2.6)$$

with

$$[J] = [\bar{J}]^{-1} \quad ; \quad [\bar{J}] = [J]^{-1} \quad ; \quad [J][\bar{J}] = [\bar{J}][J] = [I] \quad (2.7)$$

Using Murnaghan's notation

$$[J] = \frac{\partial\{\bar{x}\}}{\partial\{x\}} = \begin{bmatrix} \bar{x}_1 & \bar{x}_2 & \bar{x}_3 \\ x_1 & x_2 & x_3 \end{bmatrix} \quad ; \quad [\bar{J}] = \frac{\partial\{x\}}{\partial\{\bar{x}\}} = \begin{bmatrix} x_1 & x_2 & x_3 \\ \bar{x}_1 & \bar{x}_2 & \bar{x}_3 \end{bmatrix} \quad (2.8)$$

In 2.8 the quantities in the numerator represent rows and those in the denominator represent columns.  $[J]$  and  $[\bar{J}]$  are Jacobians of deformation. 2.5 is a co-variant transformation where as 2.6 is a contra-variant transformation. The columns of  $[J]$  are co-variant base vectors  $\tilde{\mathbf{g}}_i$  whereas the rows of  $[\bar{J}]$  are contra-variant base vectors  $\tilde{\mathbf{g}}^i$ . This distinction of rows and columns is important in defining strain measures. Thus, referring to the deformed tetrahedron, we have co-variant and contra-variant bases. The co-variant basis defines tangent vectors to the deformed material lines forming the edges of the deformed tetrahedron in the current configuration. The contra-variant basis on the other hand defines vectors with directions normal to the faces of the deformed tetrahedron formed by the co-variant base vectors.

## 2.2 Definitions and measures of stresses and strains [13]

The definitions and measures of stresses and strains in contra- and co-variant bases are of interest due to the fact that in these coordinate systems the deformed material lines are identified. If one chooses directions  $ox_1, ox_2$  and  $ox_3$  with base vectors  $\mathbf{e}_1, \mathbf{e}_2$  and  $\mathbf{e}_3$  then we can define a stress tensor  $[T]$  as

$$[T] = T_{ij} \mathbf{e}_i \mathbf{e}_j \quad (2.9)$$

On the other hand, a more natural way to define stresses is to use the current configuration (figure 2.2) and to consider the deformed volume, that is the elementary tetrahedron, with base vectors  $\tilde{\mathbf{g}}^i$  whose directions are normal to the faces of the deformed tetrahedron. On each face we have a stress in the normal direction (normal stress) and the two others (shear stresses) in the remaining two directions. This description of the stress is contra-variant description or contra-variant Cauchy stress tensor  $[\bar{T}^{(0)}]$ . Using the base vectors  $\tilde{\mathbf{g}}^i$  we could easily obtain its corresponding components in  $ox_1, ox_2$  and  $ox_3$  directions (Cartesian components). Since the directions  $\tilde{\mathbf{g}}^i$  are obtained using 2.1, it is natural to expect appearance of the co-variant basis in defining the Cartesian components of  $[\bar{T}^{(0)}]$  (equation 2.10). The contra-variant Cauchy stress definition corresponds to the faces of the actual deformed tetrahedron and hence has physical basis.

$$[T]^t = |J| [J]^{-1} [\bar{T}^{(0)}] [J]^t = [T] \quad (2.10)$$

Using 2.7 we can also write (since co- and contra-variant bases are related)

$$[T]^t = |J| [\bar{J}] [\bar{T}^{(0)}] [\bar{J}]^t = [T] \quad (2.11)$$

Equation 2.11 is more appealing since it transforms contra-variant stress components  $[\bar{T}^{(0)}]$  into Cartesian components  $[T]$  using contra-variant base vectors (rows of  $[\bar{J}]$ ). For clarity of notation we define

$$[T] = [T]^t = |J| [\bar{J}] [\bar{T}^{(0)}] [\bar{J}]^t = [T^{[0]}] \quad (\text{Def.}) \quad (2.12)$$

where  $[T^{[0]}]$  is called Second Piola-Kirchhoff stress. If we choose to define stresses using co-variant directions, then we have co-variant Cauchy stress tensor  $[\bar{T}_{(0)}]$  and its Cartesian components  $[T_{(0)}]$  can be obtained using

$$[T] = [T]^t = |J| [J]^t [\bar{T}_{(0)}] [J] = [T_{(0)}] \quad (\text{Def.}) \quad (2.13)$$

Both 2.12 and 2.13 hold for compressible matter.

For measures of strain we consider Green's strain (a co-variant measure) and Almansi strain (a contra-variant measure). These measures naturally reduce to the well known definitions of strain in linear theory of elasticity for infinitesimal deformation. A straight forward derivation of Green's strain and Almansi strain based on undeformed and deformed line segments  $ds$  and  $d\bar{s}$  in the reference and current configurations using  $[J]$  and  $[\bar{J}]$  yield the following for Green's strain  $[\varepsilon]$  and Almansi strain  $[\bar{\varepsilon}]$ :

$$[\varepsilon] = \frac{1}{2} ([J]^t [J] - [I]) \quad (\text{Def.}) \quad (2.14)$$

in which the components of  $[\varepsilon]$  correspond to the correct dyads in the Cartesian frame (say  $x$ -frame) based on the fact that columns of  $[J]$  are co-variant base vectors. For Almansi strain we have

$$[\bar{\varepsilon}] = \frac{1}{2} ([I] - [\bar{J}]^t [\bar{J}]) \quad (2.15)$$

in which  $[\bar{\varepsilon}]$  also contains Cartesian components but, based on the fact that contra-variant base vectors are rows of  $[\bar{J}]$  and not the columns, the components of  $[\bar{\varepsilon}]$  do not correspond to the correct dyads in the Cartesian frame. To correct this situation we must use a different form of  $[\bar{J}]$  in the definition of  $[\bar{\varepsilon}]$  in which the columns are the contra-variant base vector. This of course can be done by using transpose of  $[\bar{J}]$ . Thus in 2.15  $[\bar{J}]$  must be replaced with  $[\bar{J}]^t$  which yields the following definition of Almansi strain:

$$[\bar{\varepsilon}] = \frac{1}{2} ([I] - [\bar{J}] [\bar{J}]^t) \quad (\text{Def.}) \quad (2.16)$$

The components of  $[\varepsilon]$  in 2.14 and those of  $[\bar{\varepsilon}]$  in 2.16 have the same and correct dyads. In deriving convected rates we must ensure that definitions of  $[\varepsilon]$  and  $[\bar{\varepsilon}]$  in 2.14 and 2.16 are used instead of  $[\bar{\varepsilon}]$  defined by 2.15. We note that relations 2.5 and 2.6 have the assumption that infinitesimals of order two and higher can be neglected but 2.7 holds regardless of the magnitude of deformation.

### 2.3 Convected time derivatives of the Cauchy stress tensors and strain tensors

When the mathematical models based on conservation laws in Eulerian description utilize velocities as dependent variables (as in the case of fluids), the material particle displacements are not known and strain measures can not be used in the derivation of the constitutive equations. Instead, we must utilize the velocity gradient tensor in some form. Secondly, the development of the constitutive equations must consider deformed material lines in the current configuration. Thus there arises the need to consider convected time derivatives of the conjugate stress and strain measures in the chosen basis in the development of the constitutive equations for the fluids.

#### Convected time derivatives of the Cauchy stress tensors: Incompressible matter

Let  $[\bar{T}^{(0)}]$  and  $[\bar{T}_{(0)}]$  be the Cauchy stress tensors in Eulerian description corresponding to convective (or convected) coordinate systems with contra- and co-variant bases. The convected time derivatives of the tensors  $[\bar{T}^{(0)}]$  and  $[\bar{T}_{(0)}]$  in contra- and co-variant bases are of interest as these are necessary in the development of rate constitutive equations. First, we note some important relations that are needed in the derivations of the convected time derivatives [14, 15].

$$\frac{D}{Dt}[J] = [L][J] \quad (2.17)$$

$$\text{where} \quad [L] = \frac{\partial v_i}{\partial x_j} \mathbf{e}_i \mathbf{e}_j \quad (2.18)$$

The material derivative of  $[\bar{J}]$ , i.e.,  $\frac{D}{Dt}[\bar{J}]$  can be obtained using the following identity:

$$[J][\bar{J}] = [I] \quad (2.19)$$

Taking material derivative of 2.19 (Product rule holds)

$$\frac{D}{Dt}([J][\bar{J}] + [J]\frac{D}{Dt}[\bar{J}]) = 0 \quad (2.20)$$

$$\text{or} \quad \frac{D}{Dt}[\bar{J}] = -[J]^{-1} \frac{D}{Dt}([J][\bar{J}]) \quad (2.21)$$

Substituting from 2.17 into 2.21

$$\frac{D}{Dt}[\bar{J}] = -[J]^{-1}[L][J][\bar{J}] \quad (2.22)$$

$$\frac{D}{Dt}[\bar{J}] = -[\bar{J}][L] \quad (2.23)$$

Equations 2.17 and 2.23 are the key expressions that are used in deriving convected time derivatives of the stress tensors  $[\bar{T}^{(0)}]$  and  $[\bar{T}_{(0)}]$ . For incompressible matter  $|J| = 1$ .

#### Contra-variant basis:

Consider material derivative of  $[T^{[0]}]$  given by 2.12 with  $|J| = 1$ .

$$\frac{D}{Dt}[T^{[0]}] = \frac{D}{Dt}([\bar{J}][\bar{T}^{(0)}][\bar{J}]^t) \quad (2.24)$$

$$\text{or} \quad \frac{D}{Dt}[T^{[0]}] = [\bar{J}] \frac{D}{Dt}([\bar{T}^{(0)}][\bar{J}]^t) + \frac{D}{Dt}([\bar{J}][\bar{T}^{(0)}][\bar{J}]^t + [\bar{J}][\bar{T}^{(0)}] \frac{D}{Dt}[\bar{J}]^t) \quad (2.25)$$

Substituting from 2.23 into 2.25, regrouping and factoring yields

$$\frac{D}{Dt}[T^{[0]}] = [\bar{J}] \left( \frac{D}{Dt}[\bar{T}^{(0)}] - [L][\bar{T}^{(0)}] - [\bar{T}^{(0)}][L]^t \right) [\bar{J}]^t \quad (2.26)$$

If we define

$$\frac{D}{Dt}[T^{[0]}] = [T^{[1]}] \quad (\text{Def.}) \quad (2.27)$$

$$[\bar{T}^{(1)}] = \frac{D}{Dt}[\bar{T}^{(0)}] - [L][\bar{T}^{(0)}] - [\bar{T}^{(0)}][L]^t \quad (\text{Def.}) \quad (2.28)$$

then we obtain the following from: 2.26

$$[T^{[1]}] = [\bar{J}][\bar{T}^{(1)}][\bar{J}]^t \quad (2.29)$$

where  $[\bar{T}^{(1)}]$  is the first convected time derivative of the contra-variant Cauchy stress tensor  $[\bar{T}^{(0)}]$  and hence generally referred to as contra-variant first convected time derivative or upper convected time derivative (of the contra-variant Cauchy stress tensor is implied). It is straight forward to show that one could also obtain higher order convected time derivatives of the tensor  $[\bar{T}^{(0)}]$ . For example

$$[T^{[2]}] = \frac{D}{Dt}[T^{[1]}] = [\bar{J}][\bar{T}^{(2)}][\bar{J}]^t \quad (2.30)$$

$$\text{where} \quad [\bar{T}^{(2)}] = \frac{D}{Dt}[\bar{T}^{(1)}] - [L][\bar{T}^{(1)}] - [\bar{T}^{(1)}][L]^t \quad (2.31)$$

and  $[\bar{T}^{(2)}]$  is the second convected time derivative of the contra-variant Cauchy stress tensor  $[\bar{T}^{(0)}]$ .

In general, we can write the following recursive relations that can be used to obtain convected time derivative of any desired order ‘ $k$ ’ of the contra-variant Cauchy stress tensor  $[\bar{T}^{(0)}]$  for incompressible matter:

$$\left. \begin{aligned} \frac{D}{Dt}[T^{[k-1]}] &= [T^{[k]}] \\ [T^{[k]}] &= [\bar{J}][\bar{T}^{(k)}][\bar{J}]^t \\ [\bar{T}^{(k)}] &= \frac{D}{Dt}[\bar{T}^{(k-1)}] - [L][\bar{T}^{(k-1)}] - [\bar{T}^{(k-1)}][L]^t \end{aligned} \right\} \quad k = 1, 2, \dots \quad (2.32)$$

The first upper convected time derivative is generally denoted by  $\overset{\nabla}{[T]}$  and hence

$$\overset{\nabla}{[T]} = [\bar{T}^{(1)}] \quad (2.33)$$

**Co-variant basis:**

Next we consider material derivative of the Cartesian components of the co-variant Cauchy stress tensor  $[T_{[0]}]$  given by 2.13 with  $|J| = 1$  (incompressible matter).

$$\frac{D}{Dt}[T_{[0]}] = \frac{D}{Dt}([J]^t[\bar{T}_{(0)}][J]) \quad (2.34)$$

$$\text{or} \quad \frac{D}{Dt}[T_{[0]}] = [J]^t \frac{D}{Dt}([\bar{T}_{(0)}])[J] + \frac{D}{Dt}([J]^t)[\bar{T}_{(0)}][J] + [J]^t[\bar{T}_{(0)}] \frac{D}{Dt}[J] \quad (2.35)$$

Substituting from 2.17 into 2.35, regrouping and factoring gives

$$\frac{D}{Dt}[T_{[0]}] = [J]^t \left( \frac{D}{Dt}[\bar{T}_{(0)}] + [L]^t[\bar{T}_{(0)}] + [\bar{T}_{(0)}][L] \right) [J] \quad (2.36)$$

If we define

$$\frac{D}{Dt}[T_{[0]}] = [T_{[1]}] \quad (\text{Def.}) \quad (2.37)$$

$$[\bar{T}_{(1)}] = \frac{D}{Dt}[\bar{T}_{(0)}] + [L]^t[\bar{T}_{(0)}] + [\bar{T}_{(0)}][L] \quad (\text{Def.}) \quad (2.38)$$

then we obtain the following from 2.36:

$$[T_{[1]}] = [J]^t[\bar{T}_{(1)}][J] \quad (2.39)$$

where  $[\bar{T}_{(1)}]$  is the first convected time derivative of the co-variant Cauchy stress tensor  $[\bar{T}_{(0)}]$  and hence generally referred to as co-variant first convected time derivative or lower convected time derivative (of the co-variant Cauchy stress tensor is implied). In this case also, one could show that higher order convected time derivatives of the tensor  $[\bar{T}_{(0)}]$  can be easily obtained. For example

$$[T_{[2]}] = \frac{D}{Dt}[T_{[1]}] = [J]^t[\bar{T}_{(2)}][J] \quad (2.40)$$

$$\text{where} \quad [\bar{T}_{(2)}] = \frac{D}{Dt}[\bar{T}_{(1)}] + [L]^t[\bar{T}_{(1)}] + [\bar{T}_{(1)}][L] \quad (2.41)$$

and  $[\bar{T}_{(2)}]$  is the second convected time derivative of the co-variant Cauchy stress tensor  $[\bar{T}_{(0)}]$ .

In general, we can write the following recursive relations that can be used to obtain convected time derivative of any desired order ' $k$ ' of the co-variant Cauchy stress tensor  $[\bar{T}_{(0)}]$  for incompressible matter:

$$\left. \begin{aligned} \frac{D}{Dt}[T_{[k-1]}] &= [T_{[k]}] \\ [T_{[k]}] &= [J]^t[\bar{T}_{(k)}][J] \\ [\bar{T}_{(k)}] &= \frac{D}{Dt}[\bar{T}_{(k-1)}] + [L]^t[\bar{T}_{(k-1)}] + [\bar{T}_{(k-1)}][L] \end{aligned} \right\} \quad k = 1, 2, \dots \quad (2.42)$$

The lower convected time derivative is generally denoted by  $\overset{\Delta}{[T]}$  and hence

$$\overset{\Delta}{[T]} = [\bar{T}_{(1)}] \quad (2.43)$$

The material derivative operator  $\frac{D}{Dt}$  is given by

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + (\mathbf{v} \cdot \nabla) = \frac{\partial}{\partial t} + (v_i \frac{\partial}{\partial x_i}) \quad (2.44)$$

We note that the expressions for  $[\bar{T}^{(1)}]$  and  $[\bar{T}_{(1)}]$  contain material derivative plus some more terms, so we can introduce a new notation similar to material derivative and if we drop the over bar on  $[T]$  and super and subscripts [4–8, 15–20], then using 2.28 and 2.38 we can write the following for the contra- and co-variant first convected time derivatives of the corresponding stress tensors:

$$\frac{\nabla}{Dt}[T] = \frac{D}{Dt}[T] - [L][T] - [T][L]^t \quad (2.45)$$

$$\frac{\overset{\Delta}{D}}{Dt}[T] = \frac{D}{Dt}[T] + [L]^t[T] + [T][L] \quad (2.46)$$

In 2.45 and 2.46 it is understood that  $[T]$  on the right sides of the equations are contra- and co-variant Cauchy stress tensors and the left sides are their first upper convected (contra-variant) and lower convected (co-variant) time derivatives or rates. *Hence forth, we refer to these as upper convected and lower convected stress rates.*

#### Remarks:

- (1) Based on the argument presented in the introduction, i.e., section 1, it is clear that when the strains are not infinitesimal only contra-variant description is physically justifiable. Thus in case of finite deformation resulting in finite strains, only the upper convected time derivatives (of the contra-variant Cauchy stress tensor) are physical. From 2.45 and 2.46 we clearly note the differences in the convected time derivative expressions in the two cases.
- (2) Here it suffices to point out that the expression for stress rates in 2.45 - 2.46 are not the same, hence we expect the deformation behaviors obtained by using 2.46 in the constitutive models to undoubtedly deviate from the ones resulting by the use of upper convected stress rate 2.45.

- (3) It has been demonstrated [13] theoretically as well as through model problems with accurate numerical computations using methods of approximation that indeed: (a) The use of upper convected stress rate in the constitutive models captures the right physics when the deformation is finite. (b) The use of other stress rates in the constitutive models produce spurious behaviors when the strains are no longer infinitesimal. (c) Which rate equations amongst 2.45 - 2.46 remain valid for what magnitude of deformation, is problem dependent. However, from the numerical studies presented in reference [13] some inference can be drawn regarding this.
- (4) As pointed out earlier, the lower convected stress rate is a description based on a new distorted tetrahedron from that in figure 2.2 such that the co-variant base vectors are normal to the faces of this new tetrahedron. If we consider upper convected stress rate 2.45 and add  $2[D][T] + 2[T][D]$  to the right side, then by changing the meaning of  $[T]$  to co-variant measure we can write

$$\frac{\overset{\Delta}{D}}{Dt}[T] = \frac{D}{Dt}[T] - [L][T] - [T][L]^t + 2[D][T] + 2[T][D] \quad (2.47)$$

$$[D] = \frac{1}{2}([L] + [L]^t) \quad (2.48)$$

Substituting 2.48 in 2.47 yields

$$\frac{\overset{\Delta}{D}}{Dt}[T] = \frac{D}{Dt}[T] + [L]^t[T] + [T][L] \quad (2.49)$$

which is same as 2.46. Thus, the lower convected stress rate requires further deformation or distortion of the deformed tetrahedron shown in figure 2.2. We note that the term added to the right side of 2.45 only contains  $[D]$  and not  $[W]$ , hence the rotation of the actual deformed tetrahedron in figure 2.2 is precluded. This deformed configuration of the tetrahedron used in describing the lower convected stress rate is of course non-physical when the deformation is finite.

#### ***Jaumann stress rate:***

It is straight forward to show that Jaumann stress rate is the average of the upper convected and lower convected stress rates when the velocity field in the upper convected and lower convected cases are the same which is only possible if the deformation is not finite. If we define  $[\bar{T}^{(0)}] = [\bar{T}_{(0)}] = [T^J]$  as the Jaumann stress in 2.28 and 2.38 and take their average (i.e., add and divide by two), then we obtain the following:

$$\frac{^J D}{Dt}[T^J] = \frac{D}{Dt}[T^J] - \frac{1}{2}([L] - [L]^t)[T^J] + [T^J]\frac{1}{2}([L] - [L]^t) \quad (2.50)$$

Substituting for the spin tensor  $[W]$  in terms of velocity gradients and dropping the superscript  $J$  for  $[T^J]$  in 2.50, we obtain

$$\frac{^J D}{Dt}[T] = \frac{D}{Dt}[T] - [W][T] + [T][W] \quad (2.51)$$

It is important to note that  $[T]$  on the right side of 2.51 is neither a contra- nor a co-variant description. It corresponds to an intermediate tetrahedron configuration between those that are used in contra- and co-variant descriptions. We refer to  $[T]$  as Jaumann stress tensor where  $[W] = \frac{1}{2}([L] - [L]^t)$  is the spin tensor. When the deformation is finite, this description is obviously non-physical.

It is possible to define a recursive relationship to obtain Jaumann stress rates of higher order by: (i) using the recursive relations for contra- and co-variant bases and (ii) by constructing the corresponding Jaumann rates of higher order as average of the corresponding rates in co- and contra-variant bases. For this purpose let us define  $^{(0)}\bar{T}^J = [T^J]$ . Back supper script means neither contra- nor co-variant basis. Zeros in the brackets have the usual meaning.

$$\left. \begin{aligned} \frac{D}{Dt}^{[k-1]}T^J &= [^kT^J] \\ [^{(k)}\bar{T}^J] &= \frac{D}{Dt}^{[(k-1)}\bar{T}^J] - [W][^{(k-1)}\bar{T}^J] + [^{(k-1)}\bar{T}^J][W] \end{aligned} \right\} \quad k = 1, 2, \dots \quad (2.52)$$

Equation 2.52 is valid only when the velocity fields in contra- and co-variant rates are the same. In deriving 2.52 we have also used the fact that  $\frac{1}{2}[\bar{T}^{(k)}] + [\bar{T}_{(k)}] = [^{(k)}\bar{T}^J]$ .

### Convected time derivatives of the Cauchy stress tensors: Compressible matter

Following the details in section 2.3 we consider convected time derivatives of contra-variant and co-variant Cauchy stress tensors  $[\bar{T}^{(0)}]$  and  $[\bar{T}_{(0)}]$  for compressible matter. Recalling 2.12 and 2.13

$$[T^{[0]}] = |J|[\bar{J}][\bar{T}^{(0)}][\bar{J}]^t \quad (2.53)$$

$$[T_{[0]}] = |J|[J]^t[\bar{T}_{(0)}][J] \quad (2.54)$$

#### Contra-variant basis:

Consider the material derivative of  $[T^{[0]}]$ , Cartesian components of contra-variant Cauchy stress tensor defined by 2.53.

$$\frac{D}{Dt}[T^{[0]}] = \frac{D}{Dt}(|J|[\bar{J}][\bar{T}^{(0)}][\bar{J}]^t) \quad (2.55)$$

$$= \frac{D}{Dt}(|J|)[\bar{J}][\bar{T}^{(0)}][\bar{J}]^t + |J|\frac{D}{Dt}([\bar{J}][\bar{T}^{(0)}][\bar{J}]^t + |J|[\bar{J}]\frac{D}{Dt}([\bar{T}^{(0)}][\bar{J}]^t + |J|[\bar{J}][\bar{T}^{(0)}]\frac{D}{Dt}([\bar{J}]^t) \quad (2.56)$$

Substituting from 2.23 into 2.56 and noting that [14, 15]

$$\frac{D}{Dt}|J| = |J|\text{tr}([L]) \quad (2.57)$$

and regrouping the terms in 2.56

$$\frac{D}{Dt}[T^{[0]}] = |J|[\bar{J}]\left(\frac{D}{Dt}[\bar{T}^{(0)}] - [L][\bar{T}^{(0)}] - [\bar{T}^{(0)}][L]^t + [\bar{T}^{(0)}]\text{tr}([L])\right)[\bar{J}]^t \quad (2.58)$$

If we define

$$\frac{D}{Dt}[T^{[0]}] = [T^{[1]}] \quad (\text{Def.}) \quad (2.59)$$

$$[\bar{T}^{(1)}] = \frac{D}{Dt}[\bar{T}^{(0)}] - [L][\bar{T}^{(0)}] - [\bar{T}^{(0)}][L]^t + [\bar{T}^{(0)}]\text{tr}([L]) \quad (\text{Def.}) \quad (2.60)$$

then we obtain the following from 2.58:

$$[T^{[1]}] = |J|[\bar{J}][\bar{T}^{(1)}][\bar{J}]^t \quad (2.61)$$

Here  $[\bar{T}^{(1)}]$  is the first convected time derivative of the contra-variant Cauchy stress  $[\bar{T}^{(0)}]$  or upper convected time derivative of the contra-variant Cauchy stress for compressible matter.

To obtain the second convected time derivative of the contra-variant Cauchy stress we take the material derivative of 2.61, and if we follow exactly the same steps as in the case of  $[T^{[1]}]$ , then we obtain the following:

$$[T^{[2]}] = \frac{D}{Dt}[T^{[1]}] = |J|[\bar{J}][\bar{T}^{(2)}][\bar{J}]^t \quad (2.62)$$

$$\text{where} \quad [\bar{T}^{(2)}] = \frac{D}{Dt}[\bar{T}^{(1)}] - [L][\bar{T}^{(1)}] - [\bar{T}^{(1)}][L]^t + [\bar{T}^{(1)}]\text{tr}([L]) \quad (2.63)$$

In general, we can write the following recursive relations that can be used to obtain convected time derivative of any desired order ' $k$ ' of the contra-variant Cauchy stress  $[\bar{T}^{(0)}]$  for compressible matter:

$$\left. \begin{aligned} \frac{D}{Dt}[T^{[k-1]}] &= [T^{[k]}] \\ [T^{[k]}] &= |J|[\bar{J}][\bar{T}^{(k)}][\bar{J}]^t \\ [\bar{T}^{(k)}] &= \frac{D}{Dt}[\bar{T}^{(k-1)}] - [L][\bar{T}^{(k-1)}] - [\bar{T}^{(k-1)}][L]^t + [\bar{T}^{(k-1)}]\text{tr}([L]) \end{aligned} \right\} \quad k = 1, 2, \dots \quad (2.64)$$

It is straight forward to show [14, 20, 21] that  $[\bar{T}^{(k)}]$ ;  $k = 1, 2, \dots$  are objective.

**Co-variant basis:**

Next we consider the material derivative of  $[T_{[0]}]$ , Cartesian components of the co-variant Cauchy stress tensor defined by 2.54.

$$\frac{D}{Dt}[T_{[0]}] = \frac{D}{Dt}(|J|[J]^t[\bar{T}_{(0)}][J]) \quad (2.65)$$

$$= \frac{D}{Dt}(|J|)[J]^t[\bar{T}_{(0)}][J] + |J| \frac{D}{Dt}([J]^t)[\bar{T}_{(0)}][J] + |J|[J]^t \frac{D}{Dt}([\bar{T}_{(0)}])[J] + |J|[J]^t[\bar{T}_{(0)}] \frac{D}{Dt}([J]) \quad (2.66)$$

Substituting from 2.17 and 2.57 into 2.66 and regrouping the terms

$$\frac{D}{Dt}[T_{[0]}] = |J|[J]^t \left( \frac{D}{Dt}[\bar{T}_{(0)}] + [L]^t[\bar{T}_{(0)}] + [\bar{T}_{(0)}][L] + [\bar{T}_{(0)}]\text{tr}([L]) \right) [J] \quad (2.67)$$

If we define

$$\frac{D}{Dt}[T_{[0]}] = [T_{[1]}] \quad (\text{Def.}) \quad (2.68)$$

$$\bar{T}_{(1)} = \frac{D}{Dt}[\bar{T}_{(0)}] + [L]^t[\bar{T}_{(0)}] + [\bar{T}_{(0)}][L] + [\bar{T}_{(0)}]\text{tr}([L]) \quad (\text{Def.}) \quad (2.69)$$

then we obtain the following from 2.67:

$$[T_{[1]}] = |J|[J]^t[\bar{T}_{(1)}][J] \quad (2.70)$$

where  $[\bar{T}_{(1)}]$  is the first convected time derivative of the co-variant Cauchy stress  $[\bar{T}_{(0)}]$  or lower convected time derivative of the co-variant Cauchy stress for compressible matter.

To obtain the second convected time derivative of the co-variant Cauchy stress we take the material derivative of 2.70, and if we follow exactly the same steps as in the case of  $[T_{[1]}]$ , then we obtain the following:

$$[T_{[2]}] = \frac{D}{Dt}[T_{[1]}] = |J|[J]^t[\bar{T}_{(2)}][J] \quad (2.71)$$

$$\text{where} \quad \bar{T}_{(2)} = \frac{D}{Dt}[\bar{T}_{(1)}] + [L]^t[\bar{T}_{(1)}] + [\bar{T}_{(1)}][L] + [\bar{T}_{(1)}]\text{tr}([L]) \quad (2.72)$$

In general, we can write the following recursive relations that can be used to obtain convected time derivative of any desired order ' $k$ ' of the co-variant Cauchy stress  $[\bar{T}_{(0)}]$  for compressible matter:

$$\left. \begin{aligned} \frac{D}{Dt}[T_{[k-1]}] &= [T_{[k]}] \\ [T_{[k]}] &= |J|[J]^t[\bar{T}_{(k)}][J] \\ [\bar{T}_{(k)}] &= \frac{D}{Dt}[\bar{T}_{(k-1)}] + [L]^t[\bar{T}_{(k-1)}] + [\bar{T}_{(k-1)}][L] + [\bar{T}_{(k-1)}]\text{tr}([L]) \end{aligned} \right\} \quad k = 1, 2, \dots \quad (2.73)$$

In this case also, we can show [14, 20, 21] that  $[\bar{T}_{(k)}]$ ;  $k = 1, 2, \dots$  are objective.

**Jaumann stress rate:**

As in the case of incompressible matter, here also, Jaumann rate is the average of the contra- and co-variant rates when the velocity fields in the contra- and co-variant basis are the same. Thus, following the incompressible case, we can write the following recursive relations of any desired order ' $k$ ' for Jaumann stress rates:

$$\left. \begin{aligned} \frac{D}{Dt}[[^{k-1}]T^J] &= [[^k]T^J] \\ [[^{(k)}\bar{T}^J] &= \frac{D}{Dt}[[^{(k-1)}\bar{T}^J] - [W][^{(k-1)}\bar{T}^J] + [[^{(k-1)}\bar{T}^J][W] + [[^{(k-1)}\bar{T}^J]\text{tr}([L]) \end{aligned} \right\} \quad k = 1, 2, \dots \quad (2.74)$$

Equation 2.74 is valid only when the velocity fields in contra- and co-variants rates are the same. In deriving 2.74 we have also used the fact that  $\frac{1}{2}([\bar{T}^{(k)}] + [\bar{T}_{(k)}]) = [[^{(k)}\bar{T}^J]$ .

## Convected time derivatives of the strain tensors

### Co-variant basis:

Consider Green's strains  $[\varepsilon]$ , co-variant measure, and Almansi strains  $[\bar{\varepsilon}]$ , contra-variant measure, defined by 2.14 and 2.16. Consider co-variant strain description 2.14 and take material derivative of both sides.

$$\frac{D}{Dt}[\varepsilon] = \frac{1}{2} \left( \frac{D}{Dt}([J]^t)[J] + [J]^t \frac{D}{Dt}[J] \right) \quad (2.75)$$

Substituting from 2.17 and defining  $[\gamma_{(1)}]$

$$[\gamma_{(1)}] = \frac{D}{Dt}[\varepsilon] = \frac{1}{2} ([J]^t[L]^t[J] + [J]^t[L][J]) \quad (2.76)$$

$$\text{or} \quad [\gamma_{(1)}] = \frac{D}{Dt}[\varepsilon] = [J]^t \frac{1}{2} ([L]^t + [L])[J] = [J]^t[\gamma_{(0)}][J] \quad (2.77)$$

$$\text{where} \quad [\gamma_{(0)}] = [\gamma_{(1)}] = \frac{1}{2} ([L]^t + [L]) \quad (\text{Def.}) \quad (2.78)$$

Here  $[\gamma_{(0)}]$  or  $[\gamma_{(1)}]$  is known as the first convected time derivative of the co-variant strain tensor  $[\varepsilon]$ . We can also obtain higher order convected time derivatives of  $[\varepsilon]$  using a procedure similar to that used earlier in section 2.3 for stresses using  $[\gamma_{(1)}]$ . For example consider

$$[\gamma_{(2)}] = \frac{D}{Dt}[\gamma_{(1)}] = \frac{D}{Dt}([J]^t[\gamma_{(1)}][J]) \quad (2.79)$$

$$[\gamma_{(2)}] = \frac{D}{Dt}[\gamma_{(1)}] = [J]^t \frac{D}{Dt}([\gamma_{(1)}])[J] + \frac{D}{Dt}([J]^t)[\gamma_{(1)}][J] + [J]^t[\gamma_{(1)}] \frac{D}{Dt}[J] \quad (2.80)$$

Substituting from 2.17 into 2.80, rearranging and grouping terms

$$[\gamma_{(2)}] = \frac{D}{Dt}[\gamma_{(1)}] = [J]^t \left( \frac{D}{Dt}[\gamma_{(1)}] + [L]^t[\gamma_{(1)}] + [\gamma_{(1)}][L] \right) [J] \quad (2.81)$$

If we define

$$[\gamma_{(2)}] = \frac{D}{Dt}[\gamma_{(1)}] + [L]^t[\gamma_{(1)}] + [\gamma_{(1)}][L] \quad (\text{Def.}) \quad (2.82)$$

then we obtain the following:

$$[\gamma_{(2)}] = [J]^t[\gamma_{(2)}][J] \quad (2.83)$$

where  $[\gamma_{(2)}]$  is the second convected time derivatives of the co-variant strain tensor  $[\varepsilon]$ . This procedure can be used to obtain convected time derivatives of the co-variant strain tensor  $[\varepsilon]$  of any desired order. In general we can write the following recursive relations that can be used to obtain convected time derivatives of any desired order ' $k$ ' of the Green's strain tensor  $[\varepsilon]$ :

$$\left. \begin{aligned} \frac{D}{Dt}[\gamma_{(k-1)}] &= [\gamma_{(k)}] \\ [\gamma_{(k)}] &= [J]^t[\gamma_{(k)}][J] \\ [\gamma_{(k)}] &= \frac{D}{Dt}[\gamma_{(k-1)}] + [L]^t[\gamma_{(k-1)}] + [\gamma_{(k-1)}][L] \end{aligned} \right\} \quad k = 2, 3, \dots \quad (2.84)$$

with

$$[\gamma_{(1)}] = \frac{D}{Dt}[\varepsilon] = [J]^t[\gamma_{(1)}][J] \quad (2.85)$$

$$[\gamma_{(0)}] = [\gamma_{(1)}] = \frac{1}{2} ([L] + [L]^t) \quad (2.86)$$

**Contra-variant basis:**

Next, we consider contra-variant strain description 2.16 and take its material derivative

$$\frac{D}{Dt}[\bar{\varepsilon}] = -\frac{1}{2} \left( \frac{D}{Dt}([\bar{J}])[\bar{J}]^t + [\bar{J}] \frac{D}{Dt}[\bar{J}]^t \right) \quad (2.87)$$

Substituting from 2.23 in 2.87 and defining  $[\gamma^{[1]}]$

$$[\gamma^{[1]}] = \frac{D}{Dt}[\bar{\varepsilon}] = \frac{1}{2} ([\bar{J}][L][\bar{J}]^t + [\bar{J}][L]^t[\bar{J}]^t) \quad (2.88)$$

$$\text{or} \quad [\gamma^{[1]}] = \frac{D}{Dt}[\bar{\varepsilon}] = [\bar{J}] \frac{1}{2} ([L] + [L]^t)[\bar{J}]^t = [\bar{J}][\gamma^{(0)}][\bar{J}]^t \quad (2.89)$$

$$\text{where} \quad [\gamma^{(0)}] = [\gamma^{(1)}] = \frac{1}{2}([L] + [L]^t) \quad (\text{Def.}) \quad (2.90)$$

where  $[\gamma^{(0)}]$  or  $[\gamma^{(1)}]$  is known as the first convected time derivative of the contra-variant strain tensor  $[\bar{\varepsilon}]$ . We note that  $[\gamma^{(1)}] = [\gamma^{(1)}]$ . We can also define higher order convected time derivatives of  $[\bar{\varepsilon}]$  using a procedure similar to that used for the co-variant case. For example consider

$$[\gamma^{[2]}] = \frac{D}{Dt}[\gamma^{[1]}] = \frac{D}{Dt}([\bar{J}][\gamma^{(1)}][\bar{J}]^t) \quad (2.91)$$

$$[\gamma^{[2]}] = \frac{D}{Dt}[\gamma^{[1]}] = [\bar{J}] \frac{D}{Dt}([\gamma^{(1)}])[\bar{J}]^t + \frac{D}{Dt}([\bar{J}])[\gamma^{(1)}][\bar{J}]^t + [\bar{J}][\gamma^{(1)}] \frac{D}{Dt}[\bar{J}]^t \quad (2.92)$$

Substituting from 2.23 into 2.92, rearranging and regrouping terms

$$[\gamma^{[2]}] = \frac{D}{Dt}[\gamma^{[1]}] = [\bar{J}] \left( \frac{D}{Dt}[\gamma^{(1)}] - [L][\gamma^{(1)}] - [\gamma^{(1)}][L]^t \right) [\bar{J}]^t \quad (2.93)$$

If we define

$$[\gamma^{(2)}] = \frac{D}{Dt}[\gamma^{(1)}] - [L][\gamma^{(1)}] - [\gamma^{(1)}][L]^t \quad (\text{Def.}) \quad (2.94)$$

then we obtain

$$[\gamma^{[2]}] = [\bar{J}][\gamma^{(2)}][\bar{J}]^t \quad (2.95)$$

where  $[\gamma^{(2)}]$  is the second convected time derivatives of the contra-variant strain tensor  $[\bar{\varepsilon}]$ . This procedure can be used to obtain contra-variant convected time derivatives of tensor  $[\bar{\varepsilon}]$  of any desired order. In general we can write the following recursive relations that can be used to obtain convected time derivatives of any desired order 'k' of the Almansi strain tensor  $[\bar{\varepsilon}]$ :

$$\left. \begin{aligned} \frac{D}{Dt}[\gamma^{[k-1]}] &= [\gamma^{[k]}] \\ [\gamma^{[k]}] &= [\bar{J}][\gamma^{(k)}][\bar{J}]^t \\ [\gamma^{(k)}] &= \frac{D}{Dt}[\gamma^{(k-1)}] - [L][\gamma^{(k-1)}] - [\gamma^{(k-1)}][L]^t \end{aligned} \right\} \quad k = 2, 3, \dots \quad (2.96)$$

with

$$[\gamma^{[1]}] = \frac{D}{Dt}[\bar{\varepsilon}] = [\bar{J}][\gamma^{(1)}][\bar{J}]^t \quad (2.97)$$

$$[\gamma^{(0)}] = [\gamma^{(1)}] = \frac{1}{2}([L] + [L]^t) \quad (2.98)$$

where  $[\gamma^{(i)}]$  and  $[\gamma^{(i)}]$ ;  $i = 0, 1, \dots$  are fundamental kinematic tensors in contra- and co-variant bases. These are convected time derivatives of orders zero, one, and so on of the Green's strain and Almansi strain tensors in co- and contra-variant bases. These fundamental kinematic tensors (and others defined later) form the basis for deriving rate constitutive theory for both incompressible and compressible thermofluids.

### 3 Conservation laws

The fundamental principles of continuum mechanics are conservation of mass, balance of momenta and conservation of energy leading to continuity, momentum and energy equations. These are well known in both Lagrangian and Eulerian descriptions and hence are not repeated here. In addition to these, for all deforming matter to be in thermodynamic equilibrium, the second law of thermodynamics, i.e., entropy inequality or Clausius-Duhem inequality must be satisfied. We discuss details of entropy inequality in the following section as it plays a central and crucial role in the development of constitutive theory.

#### 3.1 Clausius-Duhem inequality in Eulerian or spatial description

From the point of view of thermodynamics, entropy inequality is a statement of irreversibility in most natural processes especially those involving dissipation of energy, i.e., conversion of mechanical energy into heat. From the point of view of continuum mechanics, Clausius-Duhem inequality contains much more information than just a statement of irreversibility. Analogous to the assumption of contact and body forces in the application of Newton's second law to a deforming volume of matter and the assumption of heat fluxes, source of energy, in the first law of thermodynamics, we can also postulate a similar statement for entropy. Consider a volume  $V$  of matter with closed boundary  $\partial V$  in the reference configuration. Upon deformation,  $V$  occupies  $\bar{V}(t)$  and  $\partial V$  occupies  $\partial\bar{V}(t)$  in the current configuration at time  $t$ .

Consider the deformed volume  $\bar{V}(t)$ . Let  $\bar{h}$  be the entropy flux between  $\bar{V}(t)$  and the volume of the matter surrounding it,  $\bar{s}$  be the source of entropy in  $\bar{V}(t)$  due to non-contacting bodies (considered per unit mass). Let there exist  $\bar{\eta}$ , the specific entropy (entropy per unit mass) for  $\bar{V}(t)$  bounded by  $\partial\bar{V}(t)$  such that its rate of increase is at least equal to that supplied to  $\bar{V}(t)$  from all sources (contacting and non-contacting bodies). That is

$$\frac{D}{Dt} \int_{\bar{V}(t)} \bar{\eta} \bar{\rho} d\bar{V} \geq \int_{\partial\bar{V}(t)} \bar{h} d\bar{s} + \int_{\bar{V}(t)} \bar{s} \bar{\rho} d\bar{V} \quad (3.1)$$

We adopt Cauchy's postulate for entropy flux  $\bar{h}$ , i.e.,  $\bar{h}$  at a point  $\bar{x}_i$  on  $\partial\bar{V}(t)$  depends upon the orientation  $\bar{\mathbf{n}}$  of  $\partial\bar{V}(t)$  at  $\bar{x}_i$ , i.e.

$$\bar{h} = -\bar{\Psi} \cdot \bar{\mathbf{n}} \quad (3.2)$$

in which  $\bar{\Psi}$  is similar to heat flux. Substituting from 3.2 into 3.1

$$\frac{D}{Dt} \int_{\bar{V}(t)} \bar{\eta} \bar{\rho} d\bar{V} \geq - \int_{\partial\bar{V}(t)} \bar{\Psi} \cdot \bar{\mathbf{n}} d\bar{s} + \int_{\bar{V}(t)} \bar{s} \bar{\rho} d\bar{V} \quad (3.3)$$

Using divergence theorem for the first term on the right side of 3.3

$$\frac{D}{Dt} \int_{\bar{V}(t)} \bar{\eta} \bar{\rho} d\bar{V} \geq - \int_{\bar{V}(t)} \bar{\Psi}_{i,i} d\bar{V} + \int_{\bar{V}(t)} \bar{s} \bar{\rho} d\bar{V} \quad (3.4)$$

Consider the left side of the inequality in 3.4 and use  $\bar{\rho} d\bar{V} = \rho dV$  (conservation of mass). Hence

$$\frac{D}{Dt} \int_{\bar{V}(t)} \bar{\eta} \bar{\rho} d\bar{V} = \frac{D}{Dt} \int_V \eta \rho dV = \int_V \frac{D}{Dt} (\eta \rho) dV \quad (3.5)$$

But

$$\frac{D}{Dt} (\eta \rho) = \eta \frac{D\rho}{Dt} + \rho \frac{D\eta}{Dt} = \rho \frac{D\eta}{Dt} \quad (3.6)$$

as  $\frac{D\rho}{Dt} = 0$ . Substituting from 3.6 into 3.5

$$\frac{D}{Dt} \int_{\bar{V}(t)} \bar{\eta} \bar{\rho} d\bar{V} = \int_V \rho \frac{D\eta}{Dt} dV = \int_V \frac{D\eta}{Dt} \rho dV = \int_{\bar{V}(t)} \bar{\rho} \frac{D\bar{\eta}}{Dt} d\bar{V} \quad (3.7)$$

Substituting from 3.7 into 3.4

$$\int_{\bar{V}(t)} \bar{\rho} \frac{D\bar{\eta}}{Dt} d\bar{V} \geq - \int_{\bar{V}(t)} \bar{\Psi}_{i,i} d\bar{V} + \int_{\bar{V}(t)} \bar{s} \bar{\rho} d\bar{V} \quad (3.8)$$

$$\text{or} \quad \int_{\bar{V}(t)} \left( \bar{\rho} \frac{D\bar{\eta}}{Dt} + \bar{\Psi}_{i,i} - \bar{s} \bar{\rho} \right) d\bar{V} \geq 0 \quad (3.9)$$

Since  $\bar{V}(t)$  is arbitrary we have

$$\bar{\rho} \frac{D\bar{\eta}}{Dt} + \bar{\Psi}_{i,i} - \bar{s} \bar{\rho} \geq 0 \quad (3.10)$$

Equation 3.10 is the most general form of the entropy inequality also known as Clausius-Duhem inequality. In continuum mechanics a different form of 3.10 is often more meaningful as well as useful. If we assume that

$$\bar{\Psi} = \frac{\bar{\mathbf{q}}^{(0)}}{\bar{\theta}} \quad ; \quad \bar{s} = \frac{\bar{r}}{\bar{\theta}} \quad (3.11)$$

where  $\bar{\theta}$  is absolute temperature (assumed to be greater than zero),  $\bar{\mathbf{q}}^{(0)}$  is the heat vector and  $\bar{r}$  is a suitable potential. Let

$$\bar{g}_i = \bar{\theta}_{,i} \quad (3.12)$$

Using the first expression in 3.11

$$\bar{\Psi}_{i,i} = \frac{\bar{q}_{i,i}^{(0)}}{\bar{\theta}} - \frac{\bar{q}_i^{(0)}}{(\bar{\theta})^2} \bar{\theta}_{,i} = \frac{\bar{q}_{i,i}^{(0)}}{\bar{\theta}} - \frac{\bar{q}_i^{(0)}}{(\bar{\theta})^2} \bar{g}_i \quad (3.13)$$

Substituting from 3.13 and the second expression in 3.11 into 3.10

$$\bar{\rho} \frac{D\bar{\eta}}{Dt} + \left( \frac{\bar{q}_{i,i}^{(0)}}{\bar{\theta}} - \frac{\bar{q}_i^{(0)}}{(\bar{\theta})^2} \bar{g}_i \right) - \frac{\bar{\rho} \bar{r}}{\bar{\theta}} \geq 0 \quad (3.14)$$

Multiply through out by  $\bar{\theta}$  (as  $\bar{\theta} > 0$ )

$$\bar{\rho} \bar{\theta} \frac{D\bar{\eta}}{Dt} + (\bar{q}_{i,i}^{(0)} - \bar{\rho} \bar{r}) - \frac{\bar{q}_i^{(0)} \bar{g}_i}{\bar{\theta}} \geq 0 \quad (3.15)$$

Equation 3.15 is the most common form of Clausius-Duhem inequality. 3.15 can be further given a different form using the energy equation. Recall the energy equation in Eulerian description ( $\bar{\sigma}_{ij}^{(0)}$  being the the contravariant Cauchy stress tensor).

$$\bar{\rho} \frac{D\bar{e}}{Dt} + (\bar{\nabla} \cdot \bar{\mathbf{q}}^{(0)} - \bar{\rho} \bar{r}) - \bar{\sigma}_{ij}^{(0)} \frac{\partial v_i}{\partial \bar{x}_j} = 0 \quad (3.16)$$

$$\therefore \quad \bar{\nabla} \cdot \bar{\mathbf{q}}^{(0)} - \bar{\rho} \bar{r} = \bar{q}_{i,i}^{(0)} - \bar{\rho} \bar{r} = -\bar{\rho} \frac{D\bar{e}}{Dt} + \bar{\sigma}_{ij}^{(0)} \frac{\partial v_i}{\partial \bar{x}_j} \quad (3.17)$$

Substituting from 3.17 into 3.15

$$\bar{\rho} \bar{\theta} \frac{D\bar{\eta}}{Dt} - \bar{\rho} \frac{D\bar{e}}{Dt} + \bar{\sigma}_{ij}^{(0)} \frac{\partial v_i}{\partial \bar{x}_j} - \frac{\bar{q}_i^{(0)} \bar{g}_i}{\bar{\theta}} \geq 0 \quad (3.18)$$

$$\text{or} \quad \bar{\rho} \left( \bar{\theta} \frac{D\bar{\eta}}{Dt} - \frac{D\bar{e}}{Dt} \right) + \bar{\sigma}_{ij}^{(0)} \frac{\partial v_i}{\partial \bar{x}_j} - \frac{\bar{q}_i^{(0)} \bar{g}_i}{\bar{\theta}} \geq 0 \quad (3.19)$$

$$\text{or} \quad \bar{\rho} \left( \frac{D\bar{e}}{Dt} - \bar{\theta} \frac{D\bar{\eta}}{Dt} \right) - \bar{\sigma}_{ij}^{(0)} \frac{\partial v_i}{\partial \bar{x}_j} + \frac{\bar{q}_i^{(0)} \bar{g}_i}{\bar{\theta}} \leq 0 \quad (3.20)$$

Let  $\Phi$  be the Helmholtz free energy density (specific Helmholtz free energy) defined by

$$\bar{\Phi} = \bar{e} - \bar{\eta}\bar{\theta} \quad (3.21)$$

$$\therefore \frac{D\bar{\Phi}}{Dt} = \frac{D\bar{e}}{Dt} - \bar{\eta}\frac{D\bar{\theta}}{Dt} - \bar{\theta}\frac{D\bar{\eta}}{Dt} \quad (3.22)$$

$$\therefore \frac{D\bar{e}}{Dt} - \bar{\theta}\frac{D\bar{\eta}}{Dt} = \frac{D\bar{\Phi}}{Dt} + \bar{\eta}\frac{D\bar{\theta}}{Dt} \quad (3.23)$$

Substituting from 3.23 into 3.20

$$\bar{\rho}\left(\frac{D\bar{\Phi}}{Dt} + \bar{\eta}\frac{D\bar{\theta}}{Dt}\right) + \frac{\bar{q}_i^{(0)}\bar{g}_i}{\bar{\theta}} - \bar{\sigma}_{ij}^{(0)}\frac{\partial v_i}{\partial \bar{x}_j} \leq 0 \quad (3.24)$$

This is known as the reduced form of Clausius-Duhem inequality in Eulerian or spatial description of motion. 3.24 plays important role in the development of constitutive equations.

### 3.2 Clausius-Duhem inequality in Lagrangian description

In this section we derive a form of 3.24 using Lagrangian description. In Lagrangian description, all quantities of interest are expressed as a function of  $x_i$ , coordinates of the material points in the reference configuration and time. We consider each term in 3.24

$$\rho = |J|\bar{\rho} \quad ; \quad [J] = \begin{bmatrix} \bar{x}_1, \bar{x}_2, \bar{x}_3 \\ x_1, x_2, x_3 \end{bmatrix} \quad (3.25)$$

$$\begin{aligned} \{\bar{q}^{(0)}\} &= [J^t]^{-1}\{q\} \\ \{\bar{g}\} &= \{\bar{\nabla}\bar{\theta}\} = [J^t]^{-1}\{\nabla\theta\} = [J^t]^{-1}\{g\} \end{aligned} \quad (3.26)$$

$$\begin{aligned} \bar{q}_i^{(0)}\bar{g}_i &= \bar{q}_i^{(0)}\bar{\theta}_{,i} = \{\bar{q}^{(0)}\}^t\{\bar{\nabla}\bar{\theta}\} = \{\bar{q}^{(0)}\}^t\{\bar{g}\} \\ \therefore \bar{q}_i^{(0)}\bar{g}_i &= \{q\}^t([J]^{-1}[J^t]^{-1})\{g\} \end{aligned} \quad (3.27)$$

The contra-variant Cauchy stress tensor  $[\sigma^{[0]}]$  and its Cartesian components are related;  $[\sigma^{[0]}]$  is, of course, the second Piola-Kirchhoff stress.

$$[\bar{\sigma}^{(0)}] = |J|^{-1}[J][\sigma^{[0]}][J]^t \quad (3.28)$$

where  $[\sigma^{[0]}]$  and the first Piola-Kirchhoff stress  $[\sigma^*]$  are related as well

$$[\sigma^*] = [\sigma^{[0]}][J]^t \quad (3.29)$$

Also recall,

$$L_{i,j} = v_{i,j} \quad ; \quad [\dot{J}] = [L][J] \quad (3.30)$$

Thus the last term on the right side of 3.24 becomes

$$\bar{\sigma}_{ij}^{(0)}v_{i,j} = \text{tr}([\bar{\sigma}^{(0)}][L]^t) = \text{tr}([\bar{\sigma}^{(0)}]^t[L]^t) \quad (3.31)$$

Substituting for  $[\bar{\sigma}^{(0)}]$  from 3.28 into 3.31

$$\bar{\sigma}_{ij}^{(0)}v_{i,j} = \text{tr}(|J|^{-1}[J][\sigma^{[0]}][J]^t[L]^t) = |J|^{-1}\text{tr}([J][\sigma^{[0]}][\dot{J}]^t) \quad (3.32)$$

Substituting from 3.25, 3.27 and 3.32 into 3.24

$$\rho|J|^{-1}\left(\frac{D\bar{\Phi}}{Dt} + \bar{\eta}\frac{D\bar{\theta}}{Dt}\right) + \frac{\{q\}^t([J]^{-1}[J^t]^{-1})\{g\}}{\bar{\theta}} - |J|^{-1}\text{tr}([J][\sigma^{[0]}][\dot{J}]^t) \leq 0 \quad (3.33)$$

Since  $\Phi = \Phi(x_i, t)$  and  $\theta = \theta(x_i, t)$

$$\frac{D\Phi}{Dt} = \frac{\partial\Phi}{\partial t} \quad ; \quad \frac{D\theta}{Dt} = \frac{\partial\theta}{\partial t} \quad (3.34)$$

Substituting from 3.34 into 3.33 and multiplying through out by  $|J|$ , we obtain

$$\rho \left( \frac{\partial\Phi}{\partial t} + \eta \frac{\partial\theta}{\partial t} \right) + \frac{|J| \{q\}^t ([J]^{-1} [J^t]^{-1}) \{g\}}{\theta} - \text{tr}([J] [\sigma^{[0]}] [\dot{J}]^t) \leq 0 \quad (3.35)$$

Equation 3.35 is the entropy inequality in Lagrangian description or material description of motion. The heat vector term can be simplified. Consider

$$[J]^{-1} [J^t]^{-1} = [\bar{J}] [\bar{J}]^t = [\bar{B}] \quad (3.36)$$

where  $[\bar{B}]$  is symmetric and positive definite. Hence

$$[\bar{B}] = [\underline{\psi}] [\underline{\lambda}] [\underline{\psi}]^t \quad (3.37)$$

in which  $[\underline{\psi}]$  contains normalized eigenvectors of  $[\bar{B}]$  and  $[\underline{\lambda}]$  is a diagonal matrix of the eigenvalues of  $[\bar{B}]$ . Since

$$[\underline{\lambda}] = [\sqrt{\underline{\lambda}}] [\sqrt{\underline{\lambda}}] \quad (3.38)$$

$$\therefore [\bar{B}] = [\underline{\psi}] [\sqrt{\underline{\lambda}}] [\sqrt{\underline{\lambda}}] [\underline{\psi}]^t \quad (3.39)$$

$$\begin{aligned} \therefore \{q\}^t ([J]^{-1} [J^t]^{-1}) \{g\} &= \{q\}^t [\bar{B}] \{g\} = (\{q\}^t [\underline{\psi}] [\sqrt{\underline{\lambda}}]) ([\sqrt{\underline{\lambda}}] [\underline{\psi}]^t \{g\}) \\ &= ([\sqrt{\underline{\lambda}}] [\underline{\psi}]^t \{q\})^t ([\sqrt{\underline{\lambda}}] [\underline{\psi}]^t \{g\}) \\ &= \{q\}^t \{g\} \end{aligned} \quad (3.40)$$

where

$$\{q\} = [\sqrt{\underline{\lambda}}] [\underline{\psi}]^t \{q\} \quad ; \quad \{g\} = [\sqrt{\underline{\lambda}}] [\underline{\psi}]^t \{g\} \quad (3.41)$$

Using 3.41 in the Lagrangian form of entropy inequality 3.35 we can write

$$\rho \left( \frac{\partial\Phi}{\partial t} + \eta \frac{\partial\theta}{\partial t} \right) + \frac{|J| \{\underline{q}\}^t \{\underline{g}\}}{\theta} - \text{tr}([J] [\sigma^{[0]}] [\dot{J}]^t) \leq 0 \quad (3.42)$$

$$\text{or} \quad \rho \left( \frac{\partial\Phi}{\partial t} + \eta \frac{\partial\theta}{\partial t} \right) + \frac{|J| \{\underline{q}\}^t \{\underline{g}\}}{\theta} - \text{tr}([\sigma^*]^t [\dot{J}]^t) \leq 0 \quad (3.43)$$

$$\text{or} \quad \rho \left( \frac{\partial\Phi}{\partial t} + \eta \frac{\partial\theta}{\partial t} \right) + \frac{|J| q_i g_i}{\theta} - \sigma_{ki}^* \dot{J}_{ik} \leq 0 \quad (3.44)$$

In this form each term is similar to the Eulerian form 3.24.

## 4 Preliminary considerations in the constitutive theory

From the entropy inequality we note that it contains stress  $\bar{\sigma}$  (contra- or co-variant Cauchy stress tensor), heat vector  $\bar{q}$  (contra- or co-variant heat vector), specific internal energy  $\bar{e}$  and entropy  $\bar{\eta}$  in Eulerian description and  $\sigma$  (first Piola-Kirchhoff stress, or second Piola-Kirchhoff stress, or Cartesian components of the co-variant Cauchy stress tensor),  $q$ ,  $e$  and  $\eta$  in Lagrangian description. The choice of  $\bar{e}$ ,  $\bar{\eta}$  or  $\bar{\Phi}$ ,  $\bar{\eta}$  in Eulerian description is a matter of preference as they are related through  $\bar{\Phi}$ . Likewise the choice of  $e$ ,  $\eta$  or  $\Phi$ ,  $\eta$  in Lagrangian description is a matter of preference as these are also related through  $\Phi$ . We consider  $\bar{\Phi}$ ,  $\bar{\eta}$  and  $\Phi$ ,  $\eta$  in the details that follow. Regardless of which dependent variables are chosen, i.e.,  $e$ ,  $\eta$  or  $\Phi$ ,  $\eta$ , the constitutive theory is unaffected as  $\Phi$  and  $e$  are related. In the work presented here we only consider homogeneous and isotropic matter in which a material point represents each material point in the entire volume. Thus, for homogeneous and isotropic matter, the constitutive relations at a point are valid for the entire volume of the matter.

## 4.1 Choice of dependent variables, independent variables and argument tensors of the dependent variables

### *Choice of dependent variables in the constitutive theory:*

For simple materials such as elastic solids, thermoelastic solids, thermoviscoelastic solids, Newtonian fluids, polymers etc. the objective of the constitutive theory is to provide a mathematical foundation for quantitatively establishing the stress field and heat vector in the deforming matter as functions of tensors that are measures of the physics of the deforming matter in the current configuration. Thus the stress tensor and heat vector are undoubtedly the dependent variables in the constitutive theory. Based on the comment made earlier we also choose  $\Phi$  and  $\eta$  (or  $\bar{\Phi}$  and  $\bar{\eta}$ ) as dependent variables in the constitutive theory.

Thus the choice of dependent variables in the constitutive theory is  $\sigma, q, \Phi, \eta$  (or  $\bar{\sigma}, \bar{q}, \bar{\Phi}, \bar{\eta}$ ). The dependent variables  $\sigma, q, \Phi, \eta$  are functions of argument tensors describing the physics of the deforming matter. At the onset we consider the principle or axiom of equipresence and take into account all possible tensors as arguments of  $\sigma, q, \Phi, \eta$ . Some of these may be ruled out at a later stage due to other considerations. Amongst all of the axioms of the constitutive theory, the axiom of equipresence, axiom of objectivity (form invariance) and the axiom of admissibility are the most important in the development of the constitutive theory.

### *Choice of independent variables: Axion of casualty: [20, 21]*

Based on the axion of casualty, motion of material particles of a volume of matter and their temperatures are self evident observable effects in every deforming matter. All others that enter into the expression of entropy generation are causes or dependent variables in the development of the constitutive theory. Based on this, the independent variables are

$$\bar{x}_i = \bar{x}_i(x_1, x_2, x_3, t) \quad ; \quad x_i = x_i(\bar{x}_1, \bar{x}_2, \bar{x}_3, t)$$

Thus  $\sigma, q, \Phi, \eta$  (or  $\bar{\sigma}, \bar{q}, \bar{\Phi}, \bar{\eta}$ ) must be expressed in terms of their argument tensors which in term are expressed in terms of  $(x_i, t)$  (or  $(\bar{x}_i, t)$ ).

### *Choice of argument tensors for the dependent variables in the constitutive theory:*

For the specific matter under consideration (ordered thermofluids in the present work) the choice of argument tensors for the dependent variables  $\sigma, q, \Phi$  and  $\eta$  in the constitutive theory consistent with the desired physics and in agreement with the axioms of the constitutive theory [20, 21] is obviously the most crucial and the most important aspect of the development of the constitutive theory. For the ordered thermofluids considered in this chapter, the details of the choices of these argument tensors are described in the subsequent sections.

## 4.2 Possible approaches to the constitutive theory

For a specific matter under consideration, once the argument tensors for  $\sigma, q, \Phi, \eta$  that are in agreement with the axioms of the constitutive theory are established, we can consider the following two possible approaches depending upon the type of matter.

### **Approach (1)**

Due to the axiom of admissibility, all constitutive equations must satisfy conservation laws. Conservation of mass, balance of momenta and conservation of energy are independent of the constitution of the matter. Their derivation assumes existence of the stress field and heat vector. Thus what remains is the second law of thermodynamics or Clausius-Duhem inequality. That is, all constitutive equations must satisfy entropy inequality. Said differently, if we use entropy inequality to derive constitutive equations then it will naturally be satisfied by the resulting relations. In continuum mechanics this is the fundamental approach for deriving constitutive equations. Using this approach it is possible:

- (a) To derive simple constitutive equations for the heat vector such as Fourier heat conduction law.

- (b) For elastic and thermoelastic solid matter, the stress field in a deforming matter can be established in Lagrangian description in terms of a chosen strain measure.
- (c) Additionally, thermodynamic and mechanical pressure can also be established as part of the constitutive theory.
- (d) When the mathematical models are derived using Eulerian descriptions, the entropy inequality only provides a mechanism for establishing mechanical and thermodynamic pressure with the additional restriction that the energy dissipation due to the deviatoric part of the Cauchy stress be positive, but provides no explicit mechanism for establishing the constitutive equations for it.
- (e) This approach of deriving constitutive theory obviously has thermodynamic basis as the constitutive theory in this case are derived using the conditions resulting from the second law of thermodynamics.

### Approach (2)

In deforming matter in which entropy inequality does not provide an explicit mechanism for deriving constitutive theory, we use an alternate approach. By examining the constitutive equations for elastic and thermoelastic solid matter in Lagrangian description derived using entropy inequality, we note that the expressions for the stress tensor are linear combinations of the combined generators [22–32] of the argument tensors. This observation suggests an approach for deriving constitutive equations in which the stress tensor is expressed as a linear combination of the combined generators of the argument tensors. The coefficients in the linear combination are functions of the combined invariants of the argument tensors and scalars, and are determined using their Taylor series expansions about the reference configuration (as in approach (1)). In this approach we do have to ensure that the energy dissipation is positive, a requirement from the entropy inequality.

This approach of deriving constitutive equations uses principles and concepts of continuum mechanics and hence has continuum mechanics foundation but lacks thermodynamic basis as these are not derived directly using entropy inequality.

### Remarks:

The two approaches listed above ((1) and (2)) provide a unified framework. We do remark that approach (1) is strictly in accordance with entropy inequality and hence has thermodynamic basis. Whereas, approach (2) has continuum mechanics foundation in the sense that it utilizes continuum mechanics concepts but can be viewed to lack thermodynamics foundation due to the fact that the constitutive equations in this case are not derived using the second law of thermodynamics or using the conditions resulting from it.

## 5 Development of the constitutive theory for ordered thermofluids

The ordered thermofluids are a larger class of incompressible and compressible fluids in which the stress tensor, heat vector, Helmholtz free energy density and specific entropy are functions of density, temperature, temperature gradient and convected time derivatives of the various orders of the strain tensor in the current configuration. The rationale for choosing density, temperature and temperature gradient are well established in the constitutive theory [20, 21]. However, the choice of the convected time derivatives of the strain tensor as argument tensors requires establishing a rationale. We consider details in the following.

Based on the principle of equipresence we consider all possible measures of deformation as arguments of  $\boldsymbol{\sigma}$ ,  $\mathbf{q}$ ,  $\Phi$  and  $\eta$  (or  $\bar{\boldsymbol{\sigma}}$ ,  $\bar{\mathbf{q}}$ ,  $\bar{\Phi}$  and  $\bar{\eta}$ ). The Jacobian of deformation  $[J]$  is fundamental in the kinematics and hence must be an argument in each of the four dependent variables. Since we are considering fluids,  $[\dot{J}]$  (time or material derivative of  $[J]$ ) must be in the argument list also. Temperature  $\theta$  is obviously an argument. In addition to these three, we also consider  $\mathbf{g}$ , the temperature gradient as an argument. Thus we have

$$\begin{aligned}
\boldsymbol{\sigma} &= \boldsymbol{\sigma}([J], [\dot{J}], \theta, \mathbf{g}) \\
\mathbf{q} &= \mathbf{q}([J], [\dot{J}], \theta, \mathbf{g}) \\
\Phi &= \Phi([J], [\dot{J}], \theta, \mathbf{g}) \\
\eta &= \eta([J], [\dot{J}], \theta, \mathbf{g})
\end{aligned} \tag{5.1}$$

If in 5.1 the independent variables are  $(x_i, t)$ , then these are Lagrangian or material description in which case  $\boldsymbol{\sigma}$  may represent first Piola-Kirchhoff stress, or second Piola-Kirchhoff stress (Cartesian components of the contra-variant Cauchy stress tensor), or Cartesian components of the co-variant Cauchy stress tensor. On the other hand, if the independent variables are  $(\bar{x}_i, t)$ , then these are Eulerian descriptions in which case  $\boldsymbol{\sigma}$  may represent contra- or co-variant Cauchy stress tensor.

## 5.1 Entropy inequality

We consider entropy inequality and  $\Phi(\cdot)$  in 5.1. Whether we consider the entropy inequality in Lagrangian or Eulerian description is immaterial due to the fact that all measures and their descriptions are transformable from one frame to the other using  $[J]$  and  $[\dot{J}]$ . For the sake of simplicity and clarity we consider entropy inequality in Lagrangian description 3.44. Using  $\Phi(\cdot)$  in 5.1

$$\frac{\partial \Phi}{\partial t} = \frac{\partial \Phi}{\partial J_{ik}} \dot{J}_{ik} + \frac{\partial \Phi}{\partial \dot{J}_{ik}} \ddot{J}_{ik} + \frac{\partial \Phi}{\partial \theta} \dot{\theta} + \frac{\partial \Phi}{\partial g_i} \dot{g}_i \tag{5.2}$$

Substituting 5.2 in 3.44

$$\rho \left( \frac{\partial \Phi}{\partial J_{ik}} \dot{J}_{ik} + \frac{\partial \Phi}{\partial \dot{J}_{ik}} \ddot{J}_{ik} + \frac{\partial \Phi}{\partial \theta} \dot{\theta} + \frac{\partial \Phi}{\partial g_i} \dot{g}_i + \eta \frac{\partial \theta}{\partial t} \right) + \frac{|J| \underline{q}_i \underline{g}_i}{\theta} - \sigma_{ki}^* \dot{J}_{ik} \leq 0 \tag{5.3}$$

$$\text{or} \quad \rho \frac{\partial \Phi}{\partial \dot{J}_{ik}} \ddot{J}_{ik} + \left( \rho \frac{\partial \Phi}{\partial J_{ik}} - \sigma_{ki}^* \right) \dot{J}_{ik} + \rho \left( \frac{\partial \Phi}{\partial \theta} + \eta \right) \dot{\theta} + \frac{|J| \underline{q}_i \underline{g}_i}{\theta} + \rho \frac{\partial \Phi}{\partial g_i} \dot{g}_i \leq 0 \tag{5.4}$$

In order for 5.4 to hold for arbitrary (but admissible)  $[\ddot{J}]$ ,  $\dot{\theta}$ ,  $\dot{\mathbf{g}}$ , the following must hold:

$$\frac{\partial \Phi}{\partial \dot{J}_{ik}} = 0 \tag{5.5}$$

$$\frac{\partial \Phi}{\partial g_i} = 0 \tag{5.6}$$

$$\frac{\partial \Phi}{\partial \theta} + \eta = 0 \tag{5.7}$$

$$\text{and} \quad \left( \rho \frac{\partial \Phi}{\partial J_{ik}} - \sigma_{ki}^* \right) \dot{J}_{ik} + \frac{|J| \underline{q}_i \underline{g}_i}{\theta} \leq 0 \tag{5.8}$$

Equations 5.5 - 5.8 are fundamental relations from the second law of thermodynamics (or entropy inequality).

### Remarks:

- (1) 5.5 implies that  $\Phi$  is not a function of  $[\dot{J}]$ .
- (2) 5.6 implies that  $\Phi$  is not a function of  $\mathbf{g}$  either.
- (3) Based on 5.7,  $\eta$  is not a dependent variable in constitutive theory as  $\eta = -\frac{\partial \Phi}{\partial \theta}$ , hence  $\eta$  is deterministic from  $\Phi$ .

(4) The inequality in the last equation 5.8 is essential in the form it is stated. For example

$$\rho \frac{\partial \Phi}{\partial J_{ik}} - \sigma_{ki}^* = 0 \quad \text{and} \quad \frac{|J| \underline{q_i g_i}}{\theta} \leq 0$$

are inappropriate due to the fact that these imply that  $[\sigma^*]$  is not a function of  $[\dot{J}]$  which is contrary to 5.1. However, 5.8 in its stated form is unable to provide us further details regarding the constitutive theory for  $[\sigma^*]$  and  $\mathbf{q}$ .

## 5.2 Stress decomposition

In order to alleviate the situation discussed in remark (4), we consider decomposition of  $[\sigma^*]$  into equilibrium stress  $[_e\sigma^*]$  and deviatoric stress  $[_d\sigma^*]$ , i.e.

$$[\sigma^*] = [_e\sigma^*] + [_d\sigma^*] \quad (5.9)$$

At this stage we can only conclude the following:

$$[_e\sigma^*] = [_e\sigma^*]([J], [0], \theta, \mathbf{g}) \quad (5.10)$$

$$[_d\sigma^*] = [_d\sigma^*]([J], [\dot{J}], \theta, \mathbf{g}) \quad (5.11)$$

That is,  $[_e\sigma^*]$  is not a function of  $[\dot{J}]$  and  $[_d\sigma^*]$  vanishes when  $[\dot{J}]$  and  $\mathbf{g}$  are zero. Substituting 5.9 into 5.8 gives

$$\left( \rho \frac{\partial \Phi}{\partial J_{ik}} - _e\sigma_{ki}^* - _d\sigma_{ki}^* \right) \dot{J}_{ik} + \frac{|J| \underline{q_i g_i}}{\theta} \leq 0 \quad (5.12)$$

Since  $\Phi$  is not a function of  $[\dot{J}]$  and neither is  $[_e\sigma^*]$  (due to 5.10), then  $[_e\sigma^*]$  must be derivable from

$$_e\sigma_{ki}^* = \rho \frac{\partial \Phi}{\partial J_{ik}} \quad (5.13)$$

Using 5.13, the inequality 5.12 reduces to

$$-_d\sigma_{ki}^* \dot{J}_{ik} + \frac{|J| \underline{q_i g_i}}{\theta} \leq 0 \quad (5.14)$$

If we assume (as done routinely to derive Fourier heat conduction law [14, 20, 21])

$$\frac{|J| \underline{q_i g_i}}{\theta} \leq 0 \quad (5.15)$$

Then 5.14 is satisfied if the following holds:

$$_d\sigma_{ki}^* \dot{J}_{ik} > 0 \quad (5.16)$$

Equation 5.16 requires that conversion of mechanical energy due to the deviatoric stress must be positive. Thus 5.9 can be written as

$$\sigma_{ij}^* = \rho \frac{\partial \Phi}{\partial J_{ki}} + _d\sigma_{ij}^*([J], [\dot{J}], \theta, \mathbf{g}) \quad (5.17)$$

Furthermore, based on 5.5 and 5.6 we can write

$$\Phi = \Phi([J], \theta) \quad (5.18)$$

$$\mathbf{q} = \mathbf{q}([J], [\dot{J}], \theta, \mathbf{g}) \quad (5.19)$$

Derivation of the Fourier heat conduction law for  $\mathbf{q}$  is straight forward based on 5.15 (see references [14, 20, 21]). A more general derivation of the constitutive equation for  $\mathbf{q}$  is considered in the subsequent sections. We consider further details of the argument tensors shown in 5.17 - 5.19.

### 5.3 Consideration of argument tensors for fluids

**Definition of a fluid [20, 21]:** A material point is referred to as fluid if the transformation of its reference frame by a unimodular (orthogonal) matrix can not be detected by its subsequent thermomechanical deformation ■.

Thus if  $x$ -frame changes to  $x'$ -frame via

$$\{x'\} = [R]\{x\} \quad (5.20)$$

$$\therefore [J'] = [J][R]^t \quad (5.21)$$

Then, based on the principle of frame invariance,

$$\Phi([J], \theta) = \Phi([J'], \theta) = \Phi([J][R]^t, \theta) \quad (5.22)$$

must hold and likewise, the principle of frame invariance must also hold for the stress tensor and heat vector. But this is only possible if  $\Phi$ , the stress tensor and heat vector depend upon  $|J|$  and not  $[J]$  due to the fact that

$$\det[J'] = \det([J][R]^t) = \det[J] \det[R]^t = \det[J] \quad (5.23)$$

is frame invariant. Furthermore, we note that

$$\begin{aligned} [\dot{J}] &= [L][J] \quad ; \quad [D] = \frac{1}{2}([L] + [L]^t) \quad ; \quad [W] = \frac{1}{2}([L] - [L]^t) \\ \therefore [L] &= [D] + [W] \quad \text{and} \quad [\dot{J}] = ([D] + [W])[J] \end{aligned} \quad (5.24)$$

Thus dependence of the stress tensor and heat vector on  $[\dot{J}]$  can be replaced by the dependence on  $|J|$ ,  $[D]$  and  $[W]$ . But  $[W]$  is pure rotation and hence dependence on  $[W]$  can be eliminated. Thus, the stress tensor and heat vector must have dependence on  $|J|$ ,  $[D]$ ,  $\theta$  and  $\mathbf{g}$ .

#### Further considerations regarding argument tensors

- (1) From conservation of mass

$$\rho = |J|\bar{\rho} \quad \text{or} \quad |J| = \frac{\rho}{\bar{\rho}} \quad (5.25)$$

in which  $\rho$  is constant (density in the reference configuration). Thus  $|J|$  can be replaced with  $1/\bar{\rho}$  or simply  $\bar{\rho}$ .

- (2) Since for fluids, Eulerian description is necessary, we have two obvious choices: contra-variant basis or co-variant basis and hence contra-variant Cauchy stress  $[\bar{\sigma}^{(0)}]$  or co-variant Cauchy stress  $[\bar{\sigma}_{(0)}]$  tensors are obvious choices in the constitutive theory.
- (3) Recalling the derivations of the convected time derivatives of Green's strain in the co-variant basis, we note that  $[D]$  is a convected time derivative of order one of the Green's strain, i.e.

$$[D] = [\gamma_{(1)}] \quad (5.26)$$

which is also the convected time derivative of order zero (by definition). Thus

$$[D] = [\gamma_{(0)}] = [\gamma_{(1)}] \quad (5.27)$$

By definition,  $[\gamma_{(0)}]$  and  $[\gamma_{(1)}]$  are fundamental kinematic tensors of order zero and one in co-variant basis based on Green's strain tensor, a co-variant measure of finite strain.

- (4) Likewise if we consider the convected time derivatives of the Almansi strain in contra-variant basis, we note that  $[D]$  is also the convected time derivative of order one of the Almansi strain, i.e.

$$[D] = [\gamma^{(1)}] \quad (5.28)$$

which is also the convected time derivative of order zero (by definition). Thus

$$[D] = [\gamma^{(0)}] = [\gamma^{(1)}] \quad (5.29)$$

By definition,  $[\gamma^{(0)}]$  and  $[\gamma^{(1)}]$  are fundamental kinematic tensors of order zero and one in contra-variant basis derived using Almansi strain tensor, a contra-variant measure of finite strain.

- (5) We have seen in section 2.3 that the convected time derivatives of order higher than one of the Green's strain tensor and Almansi strain tensor can be derived in co-variant and contra-variant bases which are fundamental kinematic tensors of various orders in the respective bases. Thus

$$[\gamma^{(j)}] \quad ; \quad j = 1, 2, \dots, n \quad (5.30)$$

$$\text{and} \quad [\gamma_{(j)}] \quad ; \quad j = 1, 2, \dots, n \quad (5.31)$$

are fundamental kinematic tensors in contra- and co-variant bases. Hence to generalize the development of the constitutive theory these must replace  $[D]$  in the argument tensors for the dependent variables.

With considerations (1) to (5), we now have finalized the dependent variables and their argument tensors in the rate constitutive theory.

### Final choice of the argument tensors

In Eulerian description, co-variant and contra-variant bases are obviously two clear choices for the development of the constitutive theory. In the following we consider these two bases and the choice of dependent variables and their argument tensors in these bases.

#### Contra-variant basis:

The conjugate pairs of the Cauchy stress tensor and fundamental kinematic tensors in the contra-variant basis are

$$[\bar{\sigma}^{(0)}] \quad , \quad [\gamma^{(j)}] \quad ; \quad j = 1, 2, \dots, n \quad (5.32)$$

and we have the following for the dependent variables in the constitutive theory:

$$\bar{\Phi} = \bar{\Phi}(\bar{\rho}(\bar{\mathbf{x}}, t), \bar{\theta}(\bar{\mathbf{x}}, t)) \quad (5.33)$$

$$[\bar{\sigma}^{(0)}] = [\bar{\sigma}^{(0)}(\bar{\rho}(\bar{\mathbf{x}}, t), [\gamma^{(j)}(\bar{\mathbf{x}}, t)]; j = 1, 2, \dots, n, \bar{\theta}(\bar{\mathbf{x}}, t), \bar{\mathbf{g}}(\bar{\mathbf{x}}, t))] \quad (5.34)$$

$$[\bar{\sigma}^{(0)}] = [{}_e\bar{\sigma}^{(0)}] + [{}_d\bar{\sigma}^{(0)}(\bar{\rho}(\bar{\mathbf{x}}, t), [\gamma^{(j)}(\bar{\mathbf{x}}, t)]; j = 1, 2, \dots, n, \bar{\theta}(\bar{\mathbf{x}}, t), \bar{\mathbf{g}}(\bar{\mathbf{x}}, t))] \quad (5.35)$$

$$\bar{\mathbf{q}}^{(0)} = \bar{\mathbf{q}}^{(0)}(\bar{\rho}(\bar{\mathbf{x}}, t), [\gamma^{(j)}(\bar{\mathbf{x}}, t)]; j = 1, 2, \dots, n, \bar{\theta}(\bar{\mathbf{x}}, t), \bar{\mathbf{g}}(\bar{\mathbf{x}}, t)) \quad (5.36)$$

$$[{}_e\sigma^*]^t = \rho \frac{\partial \Phi}{\partial [J]} \quad (5.37)$$

In 5.35, the contra-variant Cauchy stress tensor  $[\bar{\sigma}^{(0)}]$  has been decomposed into equilibrium stress tensor  $[{}_e\bar{\sigma}^{(0)}]$  and deviatoric Cauchy stress tensor  $[{}_d\bar{\sigma}^{(0)}]$ .

#### Co-variant basis:

The conjugate pairs of Cauchy stress tensor and fundamental kinematic tensors in the co-variant basis are

$$[\bar{\sigma}_{(0)}] \quad , \quad [\gamma_{(j)}] \quad ; \quad j = 1, 2, \dots, n \quad (5.38)$$

and we have the following for the dependent variables in the constitutive theory:

$$\bar{\Phi} = \bar{\Phi}(\bar{\rho}(\bar{\mathbf{x}}, t), \bar{\theta}(\bar{\mathbf{x}}, t)) \quad (5.39)$$

$$[\bar{\sigma}_{(0)}] = [\bar{\sigma}_{(0)}(\bar{\rho}(\bar{\mathbf{x}}, t), [\gamma_{(j)}(\bar{\mathbf{x}}, t)]; j = 1, 2, \dots, n, \bar{\theta}(\bar{\mathbf{x}}, t), \bar{\mathbf{g}}(\bar{\mathbf{x}}, t))] \quad (5.40)$$

$$[\bar{\sigma}_{(0)}] = [{}_e\bar{\sigma}_{(0)}] + [{}_d\bar{\sigma}_{(0)}(\bar{\rho}(\bar{\mathbf{x}}, t), [\gamma_{(j)}(\bar{\mathbf{x}}, t)]; j = 1, 2, \dots, n, \bar{\theta}(\bar{\mathbf{x}}, t), \bar{\mathbf{g}}(\bar{\mathbf{x}}, t))] \quad (5.41)$$

$$\bar{\mathbf{q}}_{(0)} = \bar{\mathbf{q}}_{(0)}(\bar{\rho}(\bar{\mathbf{x}}, t), [\gamma_{(j)}(\bar{\mathbf{x}}, t)]; j = 1, 2, \dots, n, \bar{\theta}(\bar{\mathbf{x}}, t), \bar{\mathbf{g}}(\bar{\mathbf{x}}, t)) \quad (5.42)$$

$$[{}_e\sigma^*]^t = \rho \frac{\partial \Phi}{\partial [J]} \quad (5.43)$$

In 5.41, the co-variant Cauchy stress tensor  $[\bar{\sigma}_{(0)}]$  has been decomposed into equilibrium stress tensor  $[{}_e\bar{\sigma}_{(0)}]$  and deviatoric Cauchy stress tensor  $[{}_d\bar{\sigma}_{(0)}]$ .

In the following sections we consider specific details of establishing explicit expressions for  $[{}_e\bar{\sigma}^{(0)}]$ ,  $[{}_e\bar{\sigma}_{(0)}]$  and  $[{}_d\bar{\sigma}^{(0)}]$ ,  $[{}_d\bar{\sigma}_{(0)}]$  followed by the constitutive theory for the heat vector.

#### 5.4 Equilibrium stress $[{}_e\bar{\sigma}^{(0)}]$ : compressible fluids

Consider contra-variant basis and the equilibrium stress  $[{}_e\bar{\sigma}^{(0)}]$  in 5.35. From 5.37 we note that  $[{}_e\sigma^*]$  is deterministic from  $\Phi(\cdot)$  and noting that for compressible matter

$$[{}_e\bar{\sigma}^{(0)}] = |J|^{-1} [{}_e\sigma^*]^t [J]^t \quad (5.44)$$

substituting from 5.37 into 5.44 gives

$$[{}_e\bar{\sigma}^{(0)}] = |J|^{-1} \rho \frac{\partial \Phi}{\partial [J]} [J]^t \quad (5.45)$$

Further simplification of 5.45 requires determination of  $\frac{\partial \Phi}{\partial [J]}$ . We can proceed in either of the two ways, details are presented in the following.

**First approach: Consider  $\bar{\Phi} = \bar{\Phi}(\bar{\rho}, \bar{\theta})$**

In this case we have

$$\frac{\partial \bar{\Phi}}{\partial [J]} = \frac{\partial \bar{\Phi}}{\partial \bar{\rho}} \frac{\partial \bar{\rho}}{\partial |J|} \frac{\partial |J|}{\partial [J]} \quad (5.46)$$

From conservation of mass

$$\rho = \bar{\rho}|J| \quad \text{or} \quad \bar{\rho} = \frac{\rho}{|J|} \quad (5.47)$$

$$\therefore \quad \frac{\partial \bar{\rho}}{\partial |J|} = -\frac{\rho}{|J|^2} = -\frac{\bar{\rho}}{|J|} \quad (5.48)$$

$$\text{and} \quad \frac{\partial |J|}{\partial [J]} = [J^{-1}]^t \quad (5.49)$$

Substituting from 5.48 and 5.49 into 5.46

$$\frac{\partial \bar{\Phi}}{\partial [J]} = \frac{\partial \bar{\Phi}}{\partial \bar{\rho}} \left( -\frac{\bar{\rho}}{|J|} \right) [J^{-1}]^t \quad (5.50)$$

Substituting from 5.47 and 5.50 into 5.45

$$[{}_e\bar{\sigma}^{(0)}] = \bar{\rho} \frac{\partial \bar{\Phi}}{\partial \bar{\rho}} \left( -\frac{\bar{\rho}}{|J|} \right) ([J^{-1}]^t [J]^t) \quad (5.51)$$

$$\text{or} \quad [{}_e\bar{\sigma}^{(0)}] = \bar{\rho} \frac{\partial \bar{\Phi}}{\partial \bar{\rho}} \left( -\frac{\bar{\rho}}{|J|} \right) [[J][J]^{-1}]^t = \left( -\frac{(\bar{\rho})^2}{|J|} \frac{\partial \bar{\Phi}}{\partial \bar{\rho}} \right) [I] \quad (5.52)$$

If we let

$$p(\bar{\rho}, \bar{\theta}) = -\frac{(\bar{\rho})^2}{|J|} \frac{\partial \bar{\Phi}}{\partial \bar{\rho}} \quad (5.53)$$

$$\text{Then} \quad [{}_e\bar{\sigma}^{(0)}] = p(\bar{\rho}, \bar{\theta}) [I] \quad (5.54)$$

**Second approach: Consider**  $\bar{\Phi} = \bar{\Phi}(1/\bar{\rho}, \bar{\theta})$

In this case

$$\frac{\partial \bar{\Phi}}{\partial [J]} = \frac{\partial \bar{\Phi}}{\partial (1/\bar{\rho})} \frac{\partial (1/\bar{\rho})}{\partial [J]} \frac{\partial [J]}{\partial [J]} \quad (5.55)$$

Since  $\frac{1}{\bar{\rho}} = \frac{|J|}{\rho}$  then

$$\frac{\partial (1/\bar{\rho})}{\partial [J]} = \frac{1}{\rho} \quad (5.56)$$

Substituting from 5.56 and 5.49 into 5.55

$$\frac{\partial \bar{\Phi}}{\partial [J]} = \frac{\partial \bar{\Phi}}{\partial (1/\bar{\rho})} \frac{1}{\rho} [J^{-1}]^t \quad (5.57)$$

$$\therefore [{}_e\bar{\sigma}^{(0)}] = |J|^{-1} \rho \left( \frac{\partial \bar{\Phi}}{\partial (1/\bar{\rho})} \frac{1}{\rho} [J^{-1}]^t \right) [J]^t \quad (5.58)$$

$$\text{or } [{}_e\bar{\sigma}^{(0)}] = |J|^{-1} \frac{\partial \bar{\Phi}}{\partial (1/\bar{\rho})} [[J][J]^{-1}]^t = \left( \frac{1}{|J|} \frac{\partial \bar{\Phi}}{\partial (1/\bar{\rho})} \right) [I] \quad (5.59)$$

If we let

$$p(1/\bar{\rho}, \bar{\theta}) = \frac{1}{|J|} \frac{\partial \bar{\Phi}}{\partial (1/\bar{\rho})} \quad (5.60)$$

$$\text{Then } [{}_e\bar{\sigma}^{(0)}] = p(1/\bar{\rho}, \bar{\theta}) [I] \quad (5.61)$$

Both definitions of  $p(\cdot)$  (equations 5.53 and 5.60) are admissible.

**Remarks:**

1. We note that 5.53 can be derived using 5.60.

$$\frac{\partial \bar{\Phi}}{\partial \bar{\rho}} = \frac{\partial \bar{\Phi}}{\partial (1/\bar{\rho})} \frac{\partial (1/\bar{\rho})}{\partial \bar{\rho}} = \frac{\partial \bar{\Phi}}{\partial (1/\bar{\rho})} \left( -\frac{1}{(\bar{\rho})^2} \right) \quad (5.62)$$

$$\therefore \frac{\partial \bar{\Phi}}{\partial (1/\bar{\rho})} = -(\bar{\rho})^2 \frac{\partial \bar{\Phi}}{\partial \bar{\rho}} \quad (5.63)$$

Substituting from 5.63 in 5.60

$$-\frac{(\bar{\rho})^2}{|J|} \frac{\partial \bar{\Phi}}{\partial \bar{\rho}} = p(\bar{\rho}, \bar{\theta}) \quad (5.64)$$

which is same as 5.53.

2. Thus for thermoviscous compressible fluids in contra-variant basis we have

$$[\bar{\sigma}^{(0)}] = p(\bar{\rho}, \bar{\theta}) [I] + [{}_d\bar{\sigma}^{(0)}(\bar{\rho}, [\gamma^{(j)}]; j = 1, 2, \dots, n, \bar{\theta}, \bar{\mathbf{g}})] \quad (5.65)$$

If we use co-variant basis, then 5.65 becomes

$$[\bar{\sigma}_{(0)}] = p(\bar{\rho}, \bar{\theta}) [I] + [{}_d\bar{\sigma}_{(0)}(\bar{\rho}, [\gamma_{(j)}]; j = 1, 2, \dots, n, \bar{\theta}, \bar{\mathbf{g}})] \quad (5.66)$$

3. We note that  $[{}_e\bar{\sigma}^{(0)}]$  is a contra-variant tensor, i.e., its components are in a non-orthogonal coordinate system. By considering the Cartesian components of  $[{}_e\bar{\sigma}^{(0)}]$ , i.e.,  $[{}_e\sigma^{[0]}]$  and by considering a rigid rotation of the  $\bar{x}$ -frame to  $\bar{x}'$ -frame we can show that  $[{}_e\sigma^{[0]}]$  and  $[{}_e\sigma^{[0]}]'$  in  $\bar{x}$ -frame and  $\bar{x}'$ -frame are the same [14]. Similar arguments hold for the co-variant case.
4.  $p(\bar{\rho}, \bar{\theta})$  is thermodynamic pressure and is completely deterministic from the deformation field once the Helmholtz free energy is defined. Instead of  $p(\bar{\rho}, \bar{\theta})$ , we can use  $-p(\bar{\rho}, \bar{\theta})$  in 5.65 and 5.66 if we define compressive pressure to be positive.

## 5.5 Equilibrium stress $[_e\bar{\sigma}^{(0)}]$ : incompressible fluids

For incompressible fluids  $\bar{\rho} = \rho$  implies that  $|J| = 1$ , hence  $\bar{\Phi} = \bar{\Phi}(\bar{\theta})$  and therefore  $\frac{\partial \bar{\Phi}}{\partial [J]} = 0$  (due to 5.46). Thus  $[_e\bar{\sigma}^{(0)}]$  for this case can not be determined using the procedure considered for the compressible case in section 5.4. Incompressibility condition  $|J| = 1$  must be enforced. We note that  $\bar{\rho} = \rho$  also implies that in Eulerian description  $\text{tr}([D]) = 0$  must hold. Hence for incompressible fluids

$$\text{tr}([D]) = \text{tr}([L]) = \text{tr}([\dot{J}][J]^{-1}) = \dot{J}_{ik}(J^{-1})_{ki} = 0 \quad (5.67)$$

We enforce 5.67 through entropy inequality. If 5.67 holds then

$$p \dot{J}_{ik}(J^{-1})_{ki} = p(\theta) \dot{J}_{ik}(J^{-1})_{ki} = 0 \quad (5.68)$$

must also hold, where  $p(\theta)$  is a multiplier (Lagrange multiplier). We add 5.68 to the left hand side of entropy inequality 5.4 (since 5.68 is zero, it does not change the meaning of entropy inequality) and regroup the terms and follow the details presented for the case of compressible matter to obtain (using 5.5)

$$\left( \rho \frac{\partial \Phi}{\partial J_{ik}} - {}_e\sigma_{ki}^* - {}_d\sigma_{ki}^* \right) \dot{J}_{ik} + \rho \left( \frac{\partial \Phi}{\partial \theta} + \eta \right) \dot{\theta} + \frac{|J| \underline{q}_i \underline{g}_i}{\theta} + \frac{\partial \Phi}{\partial g_i} \dot{g}_i + p(\theta) \dot{J}_{ik}(J^{-1})_{ki} \leq 0 \quad (5.69)$$

Regrouping the terms and substituting  $\rho \frac{\partial \Phi}{\partial J_{ik}} = 0$  in 5.69 gives

$$\left( p(\theta)(J^{-1})_{ki} - {}_e\sigma_{ik}^* - {}_d\sigma_{ki}^* \right) \dot{J}_{ik} + \rho \left( \frac{\partial \Phi}{\partial \theta} + \eta \right) \dot{\theta} + \frac{|J| \underline{q}_i \underline{g}_i}{\theta} + \frac{\partial \Phi}{\partial g_i} \dot{g}_i \leq 0 \quad (5.70)$$

Following the same reasoning as in the case of compressible fluids, we obtain the following (among others which are the same as those for the compressible case):

$${}_e\sigma_{ki}^* = p(\theta)(J^{-1})_{ki} \quad (5.71)$$

$$\text{and} \quad {}_d\sigma_{ki}^* \dot{J}_{ik} > 0 \quad (5.72)$$

Equation 5.71 can also be written as

$$[_e\sigma^*]^t = p(\theta)[J^t]^{-1} \quad (5.73)$$

But the contra-variant Cauchy stress and the first Piola-Kirchhoff stress are related

$$[\bar{\sigma}^{(0)}] = |J|^{-1} [\sigma^*]^t [J]^t \quad (5.74)$$

$|J| = 1$  in this case due to incompressibility, hence

$$[\bar{\sigma}^{(0)}] = [\sigma^*]^t [J]^t \quad (5.75)$$

Post multiply 5.73 by  $[J]^t$

$$[_e\sigma^*]^t [J]^t = p(\bar{\theta}) [J^t]^{-1} [J]^t = p(\bar{\theta}) [I] \quad (5.76)$$

By using 5.75 for the left side of 5.76 we obtain

$$[_e\bar{\sigma}^{(0)}] = p(\bar{\theta}) [I] \quad (5.77)$$

Thus for incompressible matter the constitutive equations for stress become

$$[\bar{\sigma}^{(0)}] = p(\bar{\theta}) [I] + [_d\bar{\sigma}^{(0)}](\gamma^{(j)}; j = 1, 2, \dots, n, \bar{\theta}, \bar{\mathbf{g}}) \quad (5.78)$$

We note that  $\bar{\rho}$  is no longer an argument of  $[_d\bar{\sigma}^{(0)}]$  due to incompressibility;  $p(\bar{\theta})$  is mechanical pressure. It is obvious that  $p(\bar{\theta})$  is not deterministic from the deformation field as it is an arbitrary Lagrange multiplier.

If we use co-variant basis, then 5.78 becomes

$$[\bar{\sigma}_{(0)}] = p(\bar{\theta}) [I] + [_d\bar{\sigma}_{(0)}](\gamma_{(j)}; j = 1, 2, \dots, n, \bar{\theta}, \bar{\mathbf{g}}) \quad (5.79)$$

## 5.6 Constitutive equations for deviatoric Cauchy stress tensor and heat vector

First, we make some remarks that are helpful in understanding the approach used for deriving the constitutive equations for the deviatoric stress.

- (1)  $[\gamma_{(j)}]$  and  $[\gamma^{(j)}]$ ;  $j = 1, 2, \dots, n$  are fundamental kinematic tensors of rank two,  $\bar{\mathbf{g}}$  is a tensor of rank one, and  $\bar{\rho}$ ,  $\bar{\theta}$  are tensors of rank zero.
- (2)  $[\gamma_{(j)}]$ ,  $[\gamma^{(j)}]$ ;  $j = 1, 2, \dots, n$  and  $\bar{\mathbf{g}}$  have their own invariants but also there exist combined invariants between them.
- (3) In the case of isotropic compressible fluids, the equilibrium stress is completely deterministic from the entropy inequality once we define Helmholtz free energy density in terms of the invariants of the chosen strain measure. This yields thermodynamic pressure  $p(\bar{\rho}, \bar{\theta})$ . In the case of isotropic incompressible liquids, the equilibrium stress is also derived from the entropy inequality, however, the equilibrium stress is not a function of the Helmholtz free energy density and thus it is not deterministic from the deformation field [2]. Furthermore, the second law of thermodynamics only restricts the dissipative energy (entropy production) due to the deviatoric stress to be positive but provides no mechanism for determining the constitutive equations for the deviatoric stress.
- (4) The theory of generators and invariants [22–32] provides a continuum mechanics foundation to derive constitutive equations for the deviatoric Cauchy stress. This theory utilizes a linear combination of the combined generators (of the same rank as the deviatoric Cauchy stress that are symmetric, i.e., generators are tensors of rank two and are symmetric) of the argument tensors of rank one and two to describe the deviatoric stress tensor field. The coefficients in the linear combinations are functions of the argument tensors of rank zero, and the combined invariants of the argument tensors of rank one and higher. These coefficients are then determined by using the Taylor series expansion of the coefficients about the reference configuration. Thus, in principle, this approach is quite straight forward.
- (5) Based on (4), the key element in the theory of generators and invariants is the determination of the minimal basis using the combined generators of the argument tensors and of course, determination of the combined invariants. For example  $[T([S])]$ , where  $[T]$  and  $[S]$  are symmetric tensors of rank two, which obey the invariance

$$[T([R][S][R]^t)] = [R][T([S])][R]^t \quad (5.80)$$

has the following form:

$$[T] = \alpha_0[I] + \alpha_1[S] + \alpha_2[S]^2 \quad (5.81)$$

where  $\alpha_0$ ,  $\alpha_1$  and  $\alpha_2$  are functions of the invariants of  $[S]$ , i.e.,  $\text{tr}([S])$ ,  $\text{tr}([S]^2)$  and  $\text{tr}([S]^3)$  called principal invariants, or the invariants  $I_s$ ,  $II_s$  and  $III_s$  from the characteristic equation of  $[S]$ . The tensors  $[I]$ ,  $[S]$ ,  $[S]^2$  are generators of the tensor  $[T]$  and form the minimal basis. If the arguments of  $[T]$  consist of more than one tensor (could be of different rank), then a linear combination like 5.81 would contain all combined generators (of the same rank as  $[T]$ ) of the argument tensors and likewise the coefficients in the linear combination would be functions of the argument tensors of rank zero and the combined invariants of the argument tensors of rank one and two. For details on the combined generators and invariants for various combinations of the argument tensors see references [22–32].

- (6) Based on the remarks presented above, we now have a basis for deriving constitutive theory for the deviatoric stress as well as the heat vector. In the following we consider contra-variant as well as co-variant bases, keeping in mind that the heat vector is a tensor of rank one and hence the combined generators of its argument tensors must also be of the same rank.

### Contra-variant basis: compressible matter

First, we consider compressible matter to derive constitutive equations for  $[_d\bar{\sigma}^{(0)}]$  and  $\bar{\mathbf{q}}^{(0)}$ . Recall that

$$[_d\bar{\sigma}^{(0)}] = [_d\bar{\sigma}^{(0)}](\bar{\rho}, [\gamma^{(j)}]; j = 1, 2, \dots, n, \bar{\theta}, \bar{\mathbf{g}}) \quad (5.82)$$

$$\bar{\mathbf{q}}^{(0)} = \bar{\mathbf{q}}^{(0)}(\bar{\rho}, [\gamma^{(j)}]; j = 1, 2, \dots, n, \bar{\theta}, \bar{\mathbf{g}}) \quad (5.83)$$

The generators in the linear combination representing  $[_d\bar{\sigma}^{(0)}]$  must be combined generators of  $[\gamma^{(j)}]$  ;  $j = 1, 2, \dots, n$  (since  $[\gamma^{(0)}] = [\gamma^{(1)}]$  ) and  $\bar{\mathbf{g}}$  in which  $[\gamma^{(j)}]$  are second order symmetric tensors and  $\bar{\mathbf{g}}$  is a tensor of rank one, and these combined generators must be of the same rank as  $[_d\bar{\sigma}^{(0)}]$ , i.e., of rank two as well as symmetric. In the case of  $\bar{\mathbf{q}}^{(0)}$ , a tensor of rank one, we need combined generators of  $[\gamma^{(j)}]$  ;  $j = 1, 2, \dots, n$  and  $\bar{\mathbf{g}}$  of rank one to represent  $\bar{\mathbf{q}}^{(0)}$  as a linear combination of these generators. In the derivations presented in the following we limit the argument tensors  $[\gamma^{(j)}]$  ;  $j = 1, 2, \dots, n$  to just the first two, i.e., we only consider  $[\gamma^{(1)}]$  and  $[\gamma^{(2)}]$  (generalization to more tensors presents no difficulty but the details become more involved) defining the fluid of order two. Hence

$$[_d\bar{\sigma}^{(0)}] = [_d\bar{\sigma}^{(0)}](\bar{\rho}, [\gamma^{(1)}], [\gamma^{(2)}], \bar{\theta}, \bar{\mathbf{g}}) \quad (5.84)$$

$$\bar{\mathbf{q}}^{(0)} = \bar{\mathbf{q}}^{(0)}(\bar{\rho}, [\gamma^{(1)}], [\gamma^{(2)}], \bar{\theta}, \bar{\mathbf{g}}) \quad (5.85)$$

### Constitutive equation for the stress tensor $[_d\bar{\sigma}^{(0)}]$ : Compressible fluid

First we list the combined generators [20–32] (table 2.1) and invariants [20–32] (table 2.2) for  $[_d\bar{\sigma}^{(0)}]$ . The combined generators are symmetric tensors of rank two. The combined invariants are tensors of rank zero.

Table 2.1: Combined generators for  $[_d\bar{\sigma}^{(0)}]$

Arguments	Generators
(1) none	$[I]$
(2) one at a time ( including (1) )	
$[\gamma^{(1)}]$	$[\sigma G^1] = [\gamma^{(1)}] \quad ; \quad [\sigma G^2] = [\gamma^{(1)}]^2$
$[\gamma^{(2)}]$	$[\sigma G^3] = [\gamma^{(2)}] \quad ; \quad [\sigma G^4] = [\gamma^{(2)}]^2$
$\bar{\mathbf{g}}$	$[\sigma G^5] = \bar{\mathbf{g}} \otimes \bar{\mathbf{g}}$
(3) two at a time ( including (1) and (2) )	
$[\gamma^{(1)}] \quad , \quad [\gamma^{(2)}]$	$[\sigma G^6] = [\gamma^{(1)}][\gamma^{(2)}] + [\gamma^{(2)}][\gamma^{(1)}]$ $[\sigma G^7] = [\gamma^{(1)}]^2[\gamma^{(2)}] + [\gamma^{(2)}][\gamma^{(1)}]^2$ $[\sigma G^8] = [\gamma^{(1)}][\gamma^{(2)}]^2 + [\gamma^{(2)}]^2[\gamma^{(1)}]$
$[\gamma^{(1)}] \quad , \quad \bar{\mathbf{g}}$	$[\sigma G^9] = \bar{\mathbf{g}} \otimes [\gamma^{(1)}]\bar{\mathbf{g}} + [\gamma^{(1)}]\bar{\mathbf{g}} \otimes \bar{\mathbf{g}}$ $[\sigma G^{10}] = \bar{\mathbf{g}} \otimes [\gamma^{(1)}]^2\bar{\mathbf{g}} + [\gamma^{(1)}]^2\bar{\mathbf{g}} \otimes \bar{\mathbf{g}}$
$[\gamma^{(2)}] \quad , \quad \bar{\mathbf{g}}$	$[\sigma G^{11}] = \bar{\mathbf{g}} \otimes [\gamma^{(2)}]\bar{\mathbf{g}} + [\gamma^{(2)}]\bar{\mathbf{g}} \otimes \bar{\mathbf{g}}$ $[\sigma G^{12}] = \bar{\mathbf{g}} \otimes [\gamma^{(2)}]^2\bar{\mathbf{g}} + [\gamma^{(2)}]^2\bar{\mathbf{g}} \otimes \bar{\mathbf{g}}$

**Remarks:**

- (i) We note that the invariants listed in table 2.2 under (2) ( marked (a) ) need no be included due to the fact that

$$\text{tr}([\gamma^{(1)}][\gamma^{(2)}] + [\gamma^{(2)}][\gamma^{(1)}]) + \text{tr}([\gamma^{(1)}][\gamma^{(2)}] - [\gamma^{(2)}][\gamma^{(1)}]) = 2\text{tr}([\gamma^{(1)}][\gamma^{(2)}])$$

which is same as  $q\sigma \widetilde{I}^8$  (except the factor 2, which is of no consequence). In many published works (a) are also included in addition to  $q\sigma \widetilde{I}^8$  which is redundant [14].

- (ii) Likewise, in many published works the invariant  $q\sigma \widetilde{I}^{16}$  is replaced with the two invariants listed under item (3) ( marked (b) ). Following (i), the sum of the invariants marked (b) is two times  $q\sigma \widetilde{I}^{16}$ . Hence including these in place of  $q\sigma \widetilde{I}^{16}$  is inappropriate as well.

Table 2.2: Combined invariants for  $[_d\bar{\sigma}^{(0)}]$ : These are also valid for the heat vector  $\bar{\mathbf{g}}^{(0)}$

Arguments	Invariants
<hr/>	
(1) one at a time	
$[\gamma^{(1)}]$	$q\sigma \widetilde{I}^1 = \text{tr}([\gamma^{(1)}])$ ; $q\sigma \widetilde{I}^2 = \text{tr}([\gamma^{(1)}]^2)$ $q\sigma \widetilde{I}^3 = \text{tr}([\gamma^{(1)}]^3)$
$[\gamma^{(2)}]$	$q\sigma \widetilde{I}^4 = \text{tr}([\gamma^{(2)}])$ ; $q\sigma \widetilde{I}^5 = \text{tr}([\gamma^{(2)}]^2)$ $q\sigma \widetilde{I}^6 = \text{tr}([\gamma^{(2)}]^3)$
$\bar{\mathbf{g}}$	$q\sigma \widetilde{I}^7 = \bar{\mathbf{g}} \cdot \bar{\mathbf{g}}$
<hr/>	
(2) two at a time ( including (1) )	
$[\gamma^{(1)}]$ , $[\gamma^{(2)}]$	$q\sigma \widetilde{I}^8 = \text{tr}([\gamma^{(1)}][\gamma^{(2)}])$ ; $q\sigma \widetilde{I}^9 = \text{tr}([\gamma^{(1)}]^2[\gamma^{(2)}])$ $q\sigma \widetilde{I}^{10} = \text{tr}([\gamma^{(1)}][\gamma^{(2)}]^2)$ ; $q\sigma \widetilde{I}^{11} = \text{tr}([\gamma^{(1)}]^2[\gamma^{(2)}]^2)$
	(a) $\begin{cases} q\sigma \widetilde{I} = \text{tr}([\gamma^{(1)}][\gamma^{(2)}] + [\gamma^{(2)}][\gamma^{(1)}]) \\ q\sigma \widetilde{I} = \text{tr}([\gamma^{(1)}][\gamma^{(2)}] - [\gamma^{(2)}][\gamma^{(1)}]) \end{cases}$
$[\gamma^{(1)}]$ , $\bar{\mathbf{g}}$	$q\sigma \widetilde{I}^{12} = \bar{\mathbf{g}} \cdot [\gamma^{(1)}] \bar{\mathbf{g}}$ ; $q\sigma \widetilde{I}^{13} = \bar{\mathbf{g}} \cdot [\gamma^{(1)}]^2 \bar{\mathbf{g}}$
$[\gamma^{(2)}]$ , $\bar{\mathbf{g}}$	$q\sigma \widetilde{I}^{14} = \bar{\mathbf{g}} \cdot [\gamma^{(2)}] \bar{\mathbf{g}}$ ; $q\sigma \widetilde{I}^{15} = \bar{\mathbf{g}} \cdot [\gamma^{(2)}]^2 \bar{\mathbf{g}}$
(3) three at a time ( including (1) and(2) )	
$[\gamma^{(1)}]$ , $[\gamma^{(2)}]$ , $\bar{\mathbf{g}}$	$q\sigma \widetilde{I}^{16} = \bar{\mathbf{g}} \cdot [\gamma^{(1)}][\gamma^{(2)}] \bar{\mathbf{g}}$
	(b) $\begin{cases} q\sigma \widetilde{I} = \bar{\mathbf{g}} \cdot [[\gamma^{(1)}][\gamma^{(2)}] + [\gamma^{(2)}][\gamma^{(1)}]] \bar{\mathbf{g}} \\ q\sigma \widetilde{I} = \bar{\mathbf{g}} \cdot [[\gamma^{(1)}][\gamma^{(2)}] - [\gamma^{(2)}][\gamma^{(1)}]] \bar{\mathbf{g}} \end{cases}$
<hr/>	

Now we can express  $[_d\bar{\sigma}^{(0)}]$  as a linear combination of  $[I]$  and the combined generators  $[\sigma\tilde{G}^i]$ ;  $i = 1, 2, \dots, 12$ .

$$[_d\bar{\sigma}^{(0)}] = \sigma\alpha^0[I] + \sum_{i=1}^{12} \sigma\alpha^i[\sigma\tilde{G}^i] \quad (5.86)$$

The coefficients  $\sigma\alpha^i$ ;  $i = 0, 1, \dots, 12$  are functions of the combined invariants  ${}^{q\sigma}\tilde{I}^j$ ;  $j = 1, 2, \dots, 16$ , density  $\bar{\rho}$  and temperature  $\bar{\theta}$ . The coefficients  $\sigma\alpha^i$ ;  $i = 0, 1, \dots, 12$  are determined by using Taylor series expansion for each  $\sigma\alpha^i$  about the reference configuration and only retaining up to linear terms in the combined invariants and temperature.

$$\sigma\alpha^i = \sigma\alpha^i \Big|_{\text{ref}} + \sum_{j=1}^{16} \frac{\partial(\sigma\alpha^i)}{\partial({}^{q\sigma}\tilde{I}^j)} \Big|_{\text{ref}} ({}^{q\sigma}\tilde{I}^j - ({}^{q\sigma}\tilde{I}^j)_0) + \frac{\partial(\sigma\alpha^i)}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 0, 1, \dots, 12 \quad (5.87)$$

in which the quantities with the subscript zero are their values in the reference configuration. We note that  $({}^{q\sigma}\tilde{I}^j)_0$ ;  $j = 1, 2, \dots, 16$  are all zero due to the fact that  $[\gamma^{(1)}]$  and  $[\gamma^{(2)}]$  are null in the reference configuration (fluid at rest, i.e., no motion) and  $\bar{\mathbf{g}}|_0 = 0$  if the fluid only has uniform temperature field. Hence 5.87 can be written as

$$\sigma\alpha^i = \sigma\alpha^i \Big|_{\text{ref}} + \sum_{j=1}^{16} \frac{\partial(\sigma\alpha^i)}{\partial({}^{q\sigma}\tilde{I}^j)} \Big|_{\text{ref}} {}^{q\sigma}\tilde{I}^j + \frac{\partial(\sigma\alpha^i)}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 0, 1, \dots, 12 \quad (5.88)$$

Substituting 5.88 into 5.86 gives the most general form of the constitutive relations for  $[_d\bar{\sigma}^{(0)}]$  for thermoviscous compressible fluids of order two in contra-variant basis. The final set of constants (or coefficients) resulting in this expression for the constitutive equations for  $[_d\bar{\sigma}^{(0)}]$  must be determined experimentally.

### Constitutive equation for the heat vector $\bar{\mathbf{q}}^{(0)}$ : Compressible fluid

Just like in the case of  $[_d\bar{\sigma}^{(0)}]$ , here also we need to determine the combined generators and invariants, keeping in mind that  $\bar{\mathbf{g}}$  is a tensor of rank one, hence the generators [20–32] must also be tensors of rank one (table 2.3) and that the combined invariants of the argument tensors of rank one and two for  $\bar{\mathbf{q}}^{(0)}$  are the same as those for  $[_d\bar{\sigma}^{(0)}]$  (already defined in table 2.2).

Now we can express  $\bar{\mathbf{q}}^{(0)}$  as a linear combination of the combined generators  $\{q\tilde{G}^i\}$ ;  $i = 1, 2, \dots, 7$  in the contra-variant basis.

$$\bar{\mathbf{q}}^{(0)} = - \sum_{i=1}^7 q\alpha^i \{q\tilde{G}^i\} \quad (5.89)$$

The coefficients  $q\alpha^i$ ;  $i = 1, 2, \dots, 7$  are functions of the combined invariants  ${}^{q\sigma}\tilde{I}^j$ ;  $j = 1, 2, \dots, 16$ , density  $\bar{\rho}$  and temperature  $\bar{\theta}$ . The coefficients  $q\alpha^i$ ;  $i = 1, 2, \dots, 7$  are determined by using Taylor series expansion for each  $q\alpha^i$  about the reference configuration and retaining only up to linear terms in the combined invariants and temperature.

$$q\alpha^i = q\alpha^i \Big|_{\text{ref}} + \sum_{j=1}^{16} \frac{\partial(q\alpha^i)}{\partial({}^{q\sigma}\tilde{I}^j)} \Big|_{\text{ref}} ({}^{q\sigma}\tilde{I}^j - ({}^{q\sigma}\tilde{I}^j)_0) + \frac{\partial(q\alpha^i)}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 1, 2, \dots, 7 \quad (5.90)$$

in which the quantities with the subscript zero are their values in the reference configuration. As before,  $({}^{q\sigma}\tilde{I}^j)_0$ ;  $j = 1, 2, \dots, 16$  are all zero, and if  $\bar{\mathbf{g}}|_0 = 0$ , then 5.90 reduces to

$$q\alpha^i = q\alpha^i \Big|_{\text{ref}} + \sum_{j=1}^{16} \frac{\partial(q\alpha^i)}{\partial({}^{q\sigma}\tilde{I}^j)} \Big|_{\text{ref}} {}^{q\sigma}\tilde{I}^j + \frac{\partial(q\alpha^i)}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 1, 2, \dots, 7 \quad (5.91)$$

Substituting 5.91 in 5.89 gives the most general form of the constitutive equation for the heat vector  $\bar{\mathbf{q}}^{(0)}$  for thermoviscous compressible fluids in contra-variant basis. The final set of constants (or coefficients) appearing in the constitutive equation for  $\bar{\mathbf{q}}^{(0)}$  must be determined experimentally.

Table 2.3: Combined generators for  $\bar{\mathbf{q}}^{(0)}$ 

Arguments	Generators
(1) one at a time	
$[\gamma^{(1)}]$	none
$[\gamma^{(2)}]$	none
$\bar{\mathbf{g}}$	$\{^q\tilde{G}^1\} = \bar{\mathbf{g}}$
(2) two at a time ( including (1) )	
$[\gamma^{(1)}]$ , $[\gamma^{(2)}]$	none
$[\gamma^{(1)}]$ , $\bar{\mathbf{g}}$	$\{^q\tilde{G}^2\} = [\gamma^{(1)}] \bar{\mathbf{g}}$ $\{^q\tilde{G}^3\} = [\gamma^{(1)}]^2 \bar{\mathbf{g}}$
$[\gamma^{(2)}]$ , $\bar{\mathbf{g}}$	$\{^q\tilde{G}^4\} = [\gamma^{(2)}] \bar{\mathbf{g}}$ $\{^q\tilde{G}^5\} = [\gamma^{(2)}]^2 \bar{\mathbf{g}}$
(3) three at a time ( including (1) and (2) )	
$[\gamma^{(1)}]$ , $[\gamma^{(2)}]$ , $\bar{\mathbf{g}}$	$\{^q\tilde{G}^6\} = [[\gamma^{(1)}][\gamma^{(2)}] + [\gamma^{(2)}][\gamma^{(1)}]] \bar{\mathbf{g}}$ $\{^q\tilde{G}^7\} = [[\gamma^{(1)}][\gamma^{(2)}] - [\gamma^{(2)}][\gamma^{(1)}]] \bar{\mathbf{g}}$

The constitutive equations presented so far for  $[_d\bar{\sigma}^{(0)}]$  and  $\bar{\mathbf{q}}^{(0)}$  are the most general form of the constitutive equations for thermoviscous compressible fluids of order two in contra-variant basis. It is possible to derive the constitutive equations for the deviatoric stress and heat vector in co-variant basis also following exactly the same steps as used for contra-variant basis but making appropriate modifications due to the change of basis from contra- to co-variant. Details are presented in the following.

### Co-variant basis: compressible matter

In co-variant basis we have

$$[_d\bar{\sigma}_{(0)}] = [_d\bar{\sigma}_{(0)}](\bar{\rho}, [\gamma_{(j)}]; j = 1, 2, \dots, n, \bar{\theta}, \bar{\mathbf{g}}) \quad (5.92)$$

$$\bar{\mathbf{q}}_{(0)} = \bar{\mathbf{q}}_{(0)}(\bar{\rho}, [\gamma_{(j)}]; j = 1, 2, \dots, n, \bar{\theta}, \bar{\mathbf{g}}) \quad (5.93)$$

where  $[\gamma_{(j)}]$  are fundamental kinematic tensors in co-variant basis. As in the contra-variant case, here also, if we limit the kinematic tensors to just the first two, i.e.,  $[\gamma_{(1)}]$  and  $[\gamma_{(2)}]$ , then we have

$$[_d\bar{\sigma}_{(0)}] = [_d\bar{\sigma}_{(0)}](\bar{\rho}, [\gamma_{(1)}], [\gamma_{(2)}], \bar{\theta}, \bar{\mathbf{g}}) \quad (5.94)$$

$$\bar{\mathbf{q}}_{(0)} = \bar{\mathbf{q}}_{(0)}(\bar{\rho}, [\gamma_{(1)}], [\gamma_{(2)}], \bar{\theta}, \bar{\mathbf{g}}) \quad (5.95)$$

We use 5.94 and 5.95 to present the remaining details.

### Constitutive equation for the stress tensor $[d\bar{\sigma}_{(0)}]$ : Compressible fluid

In this case we expect a total of twelve combined generators (as in the contra-variant case). Let us define these as  $[\sigma G_i]$ ;  $i = 1, 2, \dots, 12$ . These can be obtained using the definitions of  $[\sigma G_i]$ ;  $i = 1, 2, \dots, 12$  but replacing  $[\gamma^{(1)}]$  and  $[\gamma^{(2)}]$  with  $[\gamma_{(1)}]$  and  $[\gamma_{(2)}]$ . Likewise the combined invariants  ${}^{q\sigma}\tilde{I}_i$ ;  $i = 1, 2, \dots, 16$  can be obtained from  ${}^{q\sigma}\tilde{I}_i$ ;  $i = 1, 2, \dots, 16$  by replacing  $[\gamma^{(1)}]$  and  $[\gamma^{(2)}]$  with  $[\gamma_{(1)}]$  and  $[\gamma_{(2)}]$ .

Now, we can express  $[d\bar{\sigma}_{(0)}]$  as a linear combination of  $[I]$  and the combined generators  $[\sigma G_i]$ ;  $i = 1, 2, \dots, 12$  in the co-variant basis.

$$[d\bar{\sigma}_{(0)}] = \sigma_{\alpha_0}[I] + \sum_{i=1}^{12} \sigma_{\alpha_i}[\sigma G_i] \quad (5.96)$$

The coefficients  $\sigma_{\alpha_i}$ ;  $i = 0, 1, \dots, 12$  are functions of the combined invariants  ${}^{q\sigma}\tilde{I}_j$ ;  $j = 1, 2, \dots, 16$ , density  $\bar{\rho}$  and temperature  $\bar{\theta}$ . The coefficients  $\sigma_{\alpha_i}$ ;  $i = 0, 1, \dots, 12$  are determined by using Taylor series expansion for each  $\sigma_{\alpha_i}$  about the reference configuration and only retaining up to linear terms in the combined invariants and temperature.

$$\sigma_{\alpha_i} = \sigma_{\alpha_i} \Big|_{\text{ref}} + \sum_{j=1}^{16} \frac{\partial(\sigma_{\alpha_i})}{\partial({}^{q\sigma}\tilde{I}_j)} \Big|_{\text{ref}} ({}^{q\sigma}\tilde{I}_j - ({}^{q\sigma}\tilde{I}_j)_0) + \frac{\partial(\sigma_{\alpha_i})}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 0, 1, \dots, 12 \quad (5.97)$$

in which quantities with subscript zero are their values in the reference configuration. Since  $({}^{q\sigma}\tilde{I}_j)_0$ ;  $j = 1, 2, \dots, 16$  are all zero (for the same reasons as in the contra-variant case) and if  $\bar{\mathbf{g}}|_0 = 0$  then 5.97 reduces to

$$\sigma_{\alpha_i} = \sigma_{\alpha_i} \Big|_{\text{ref}} + \sum_{j=1}^{16} \frac{\partial(\sigma_{\alpha_i})}{\partial({}^{q\sigma}\tilde{I}_j)} \Big|_{\text{ref}} {}^{q\sigma}\tilde{I}_j + \frac{\partial(\sigma_{\alpha_i})}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 0, 1, \dots, 12 \quad (5.98)$$

By substituting from 5.98 into 5.96, we obtain the most general form of the constitutive equations for  $[d\bar{\sigma}_{(0)}]$  for thermoviscous compressible fluids of order two in co-variant basis. Here also, the final set of constants (or coefficients) resulting in this expression must be determined experimentally.

### Constitutive equation for the heat vector $\bar{\mathbf{q}}_{(0)}$ : Compressible fluid

In this case also (as in contra-variant basis) we have seven combined generators  $\{{}^qG_i\}$ ;  $i = 1, 2, \dots, 7$  and the combined invariants remain the same as for  $[d\bar{\sigma}_{(0)}]$ , i.e., same as  ${}^{q\sigma}\tilde{I}_i$ ;  $i = 1, 2, \dots, 16$ . The combined generators  $\{{}^qG_i\}$ ;  $i = 1, 2, \dots, 7$  can be obtained from  $\{{}^qG_i\}$ ;  $i = 1, 2, \dots, 7$  by replacing  $[\gamma^{(1)}]$  and  $[\gamma^{(2)}]$  with  $[\gamma_{(1)}]$  and  $[\gamma_{(2)}]$ . Now we can express  $\bar{\mathbf{q}}_{(0)}$  as

$$\bar{\mathbf{q}}_{(0)} = - \sum_{i=1}^7 {}^q\alpha_i \{{}^qG_i\} \quad (5.99)$$

The coefficients  ${}^q\alpha_i$ ;  $i = 1, 2, \dots, 7$  are functions of the combined invariants  ${}^{q\sigma}\tilde{I}_i$ ;  $i = 1, 2, \dots, 16$ , density  $\bar{\rho}$  and temperature  $\bar{\theta}$ . The coefficients  ${}^q\alpha_i$  are determined by using Taylor series expansion for each  ${}^q\alpha_i$  about the reference configuration and retaining only up to linear terms in the combined invariants and temperature.

$${}^q\alpha_i = {}^q\alpha_i \Big|_{\text{ref}} + \sum_{j=1}^{16} \frac{\partial({}^q\alpha_i)}{\partial({}^{q\sigma}\tilde{I}_j)} \Big|_{\text{ref}} ({}^{q\sigma}\tilde{I}_j - ({}^{q\sigma}\tilde{I}_j)_0) + \frac{\partial({}^q\alpha_i)}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 1, 2, \dots, 7 \quad (5.100)$$

As before, the quantities with the subscript zero are their values in the reference configuration and  $({}^{q\sigma}\tilde{I}_j)_0$ ;  $j = 1, 2, \dots, 16$  are all zero (for the same reasons as before) and if  $\bar{\mathbf{g}}|_0 = 0$  then 5.100 can be written as

$${}^q\alpha_i = {}^q\alpha_i \Big|_{\text{ref}} + \sum_{j=1}^{16} \frac{\partial({}^q\alpha_i)}{\partial({}^{q\sigma}\tilde{I}_j)} \Big|_{\text{ref}} {}^{q\sigma}\tilde{I}_j + \frac{\partial({}^q\alpha_i)}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 1, 2, \dots, 7 \quad (5.101)$$

Substituting from 5.101 into 5.99 gives the most general form of constitutive equations for the heat vector  $\bar{\mathbf{q}}_{(0)}$  for thermoviscous compressible fluids of order two in co-variant basis. Determination of the constants (or coefficients) in this final form must be done experimentally.

## 6 Remarks regarding the constitutive theory in contra- and co-variant bases

In section 5, most general derivations of the constitutive theory for the Cauchy stress tensor and heat vector have been presented for ‘ordered thermofluids’ (order two considered to present specific details) in contra- and co-variant bases. The derivations are made specific by choosing only first and second convected time derivatives of the Green’s strain and Almansi strain in co- and contra-variant bases to present details of the constitutive equations. Inclusion of the convected time derivatives of order higher than two as argument tensors poses no special problem except that it would involve more and new combined generators and invariants. We make two important remarks.

- (1) Since  $[\gamma^{(j)}] \neq [\gamma_{(j)}]$  ;  $j = 2, 3, \dots, n$ , it is obvious that  $[_d\bar{\sigma}^{(0)}] \neq [_d\bar{\sigma}_{(0)}]$  and likewise  $\bar{\mathbf{q}}^{(0)} \neq \bar{\mathbf{q}}_{(0)}$ . That is, the constitutive equations for deviatoric stress and heat vector differ in contra- and co-variant bases.
- (2) The constitutive equation for the heat vector presented here is much more general and relatively more complex than the simple Fourier heat conduction law, which can be derived using conditions resulting from the Clausius-Duhem inequality. The constitutive equation for  $\bar{\mathbf{q}}^{(0)}$  presented here has the potential of perhaps providing a more realistic constitutive law for the heat vector for fluids with complex motion of fluid particles as opposed to the simple Fourier heat conduction law which was originally derived for solid matter.
- (3) In many practical applications involving thermofluids the constitutive theory of order one is found to describe the physics adequately. In this case, convected time derivative of order one will appear as argument tensor (in addition to density, temperature and temperature gradient) for all dependent variables in the constitutive theory (stress tensor, heat vector and Helmholtz free energy density), keeping in mind that such constitutive theory is incapable of predicting finite deformation.

In this case  $[_d\bar{\sigma}^{(0)}]$  is expressed as a linear combination of  $[I]$  and the combined generators of  $[\gamma^{(1)}]$  and  $\bar{\mathbf{g}}$  that are symmetric and are of rank two. The heat vector  $\bar{\mathbf{q}}^{(0)}$  is expressed as a linear combination of the combined generators of  $[\gamma^{(1)}]$  and  $\bar{\mathbf{g}}$  that are of rank one. The coefficients in both linear combinations are functions of  $\bar{\rho}$ ,  $\bar{\theta}$  and the combined invariants of  $[\gamma^{(1)}]$  and  $\bar{\mathbf{g}}$ . Both  $[_d\bar{\sigma}^{(0)}]$  and  $\bar{\mathbf{q}}^{(0)}$  are contra-variant descriptions. By replacing  $[\gamma^{(1)}]$  with  $[\gamma_{(1)}]$  the contra-variant description can be converted to co-variant description for the deviatoric stress tensor and heat vector. The details of these constitutive equations are presented in section 7.

- (4) Further simplifications of the constitutive theory described in remark (3) is also possible. For example, if we assume that the deviatoric stress only depends upon density, temperature and the first convected time derivative of the strain tensor (Green’s or Almansi depending upon co- or contra-variant basis) and if we also assume that the heat vector only depends upon density, temperature and temperature gradient, then we obtain a much simplified form of the constitutive equations for the deviatoric stress and heat vector in the chosen basis. From these constitutive equations we realize the well known relations for generalized Newtonian fluids for stress deviation and Fourier heat conduction law. Upon further simplifications we obtain the well known constitutive equations for Newtonian fluids for the deviatoric stress. The various forms of constitutive equations described here also describe thermoviscous fluids (but with the stated assumptions). These are obviously a subcategory of the general class of thermoviscous fluids discussed in remark (3) (thermofluids of order one). The details of the constitutive equations described here are presented in section 8.
- (5) We note that the constitutive equations for the Cauchy stresses describe the deviatoric Cauchy stress tensor (  $[_d\bar{\sigma}^{(0)}]$  or  $[_d\bar{\sigma}_{(0)}]$  ) as a function of the convected time derivatives of the strain tensor (Almansi or Green). However  $[_d\bar{\sigma}^{(0)}]$  and  $[_d\bar{\sigma}_{(0)}]$  are convected time derivatives of order zero of the contra- and co-variant Cauchy stress tensor. Thus the constitutive equations for the deviatoric Cauchy stress tensors presented here are indeed rate constitutive equations in which stress rates of order zero are functions of the convected time derivatives of the strain tensor of various orders in appropriately chosen conjugate descriptions of stress and strain measures.

## 7 Constitutive equations for thermoviscous fluids of order one

We consider both contra- and co-variant bases.

### 7.1 Contra-variant basis

In this case we have

$$[{}_d\bar{\sigma}^{(0)}] = [{}_d\bar{\sigma}^{(0)}(\bar{\rho}, [\gamma^{(1)}], \bar{\theta}, \bar{\mathbf{g}})] \quad (7.1)$$

$$\bar{\mathbf{q}}^{(0)} = \bar{\mathbf{q}}^{(0)}(\bar{\rho}, [\gamma^{(1)}], \bar{\theta}, \bar{\mathbf{g}}) \quad (7.2)$$

$$\bar{\Phi} = \bar{\Phi}(\bar{\rho}, \bar{\theta}) \quad (7.3)$$

#### Deviatoric Cauchy stress $[{}_d\bar{\sigma}^{(0)}]$

The combined generators of tensors  $[\gamma^{(1)}]$  and  $\bar{\mathbf{g}}$  that are symmetric tensors of rank 2 are (table 2.1)

$$[\sigma G^1] = [\gamma^{(1)}] \quad ; \quad [\sigma G^2] = [\gamma^{(1)}]^2 \quad ; \quad [\sigma G^3] = \bar{\mathbf{g}} \otimes \bar{\mathbf{g}} \quad (7.4)$$

The combined invariants of the tensors  $[\gamma^{(1)}]$  and  $\bar{\mathbf{g}}$  are (table 2.2)

$$\begin{aligned} {}^{q\sigma}I^1 &= \text{tr}([\gamma^{(1)}]) \quad ; \quad {}^{q\sigma}I^2 = \text{tr}([\gamma^{(1)}]^2) \quad ; \quad {}^{q\sigma}I^3 = \text{tr}([\gamma^{(1)}]^3) \\ {}^{q\sigma}I^4 &= \bar{\mathbf{g}} \cdot \bar{\mathbf{g}} \quad ; \quad {}^{q\sigma}I^5 = \bar{\mathbf{g}} \cdot [\gamma^{(1)}] \bar{\mathbf{g}} \quad ; \quad {}^{q\sigma}I^6 = \bar{\mathbf{g}} \cdot [\gamma^{(1)}]^2 \bar{\mathbf{g}} \end{aligned} \quad (7.5)$$

$$\therefore \quad [{}_d\bar{\sigma}^{(0)}] = \sigma \hat{\alpha}^0 [I] + \sum_{i=1}^3 \sigma \hat{\alpha}^i [\sigma G^i] \quad (7.6)$$

The coefficients  $\sigma \hat{\alpha}^i$  are functions of density  $\bar{\rho}$ , temperature  $\bar{\theta}$  and the combined invariants  ${}^{q\sigma}I^j$ ;  $j = 1, 2, \dots, 6$ .

These are determined by using Taylor series expansion of  $\sigma \hat{\alpha}^i$  about the reference configuration and by only retaining up to linear terms in the combined invariants and temperature.

$$\sigma \hat{\alpha}^i = \sigma \hat{\alpha}^i \Big|_{\text{ref}} + \sum_{j=1}^6 \frac{\partial(\sigma \hat{\alpha}^i)}{\partial({}^{q\sigma}I^j)} \Big|_{\text{ref}} ({}^{q\sigma}I^j - ({}^{q\sigma}I^j)_0) + \frac{\partial(\sigma \hat{\alpha}^i)}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 0, 1, \dots, 3 \quad (7.7)$$

Since  $({}^{q\sigma}I^j)_0 = 0$ ;  $j = 1, 2, \dots, 6$ , expression 7.7 reduces to

$$\sigma \hat{\alpha}^i = \sigma \hat{\alpha}^i \Big|_{\text{ref}} + \sum_{j=1}^6 \frac{\partial(\sigma \hat{\alpha}^i)}{\partial({}^{q\sigma}I^j)} \Big|_{\text{ref}} {}^{q\sigma}I^j + \frac{\partial(\sigma \hat{\alpha}^i)}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 0, 1, \dots, 3 \quad (7.8)$$

By substituting from 7.8 into 7.6 we obtain the constitutive equations for  $[{}_d\bar{\sigma}^{(0)}]$ . This is the most general form of the constitutive equations for deviatoric stress for thermofluids of order one.

#### Heat vector $\bar{\mathbf{q}}^{(0)}$

The combined generators of the tensors  $[\gamma^{(1)}]$  and  $\bar{\mathbf{g}}$  that are of rank one are (table 2.3)

$$\{{}^qG^1\} = \bar{\mathbf{g}} \quad ; \quad \{{}^qG^2\} = [\gamma^{(1)}] \bar{\mathbf{g}} \quad ; \quad \{{}^qG^3\} = [\gamma^{(1)}]^2 \bar{\mathbf{g}} \quad (7.9)$$

The combined invariants remain the same as defined by 7.5

$$\therefore \quad \bar{\mathbf{q}}^{(0)} = - \sum_{i=1}^3 {}^q\hat{\alpha}^i \{{}^qG^i\} \quad (7.10)$$

The coefficients  ${}^q\hat{\alpha}^i$  are functions of density  $\bar{\rho}$ , temperature  $\bar{\theta}$  and the combined invariants  ${}^{q\sigma}I^j$ ;  $j = 1, 2, \dots, 6$  given by 7.5. These are determined by using the Taylor series expansion of  ${}^q\hat{\alpha}^i$  about the reference configuration and by only retaining up to linear terms in the combined invariants and temperature.

$${}^q\hat{\alpha}^i = {}^q\hat{\alpha}^i \Big|_{\text{ref}} + \sum_{j=1}^6 \frac{\partial({}^q\hat{\alpha}^i)}{\partial({}^{q\sigma}I^j)} \Big|_{\text{ref}} ({}^{q\sigma}I^j - ({}^{q\sigma}I^j)_0) + \frac{\partial({}^q\hat{\alpha}^i)}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 0, 1, \dots, 3 \quad (7.11)$$

Since  $({}^{q\sigma}I^j)_{\sim 0} = 0$ ;  $j = 1, 2, \dots, 6$ , expression 7.11 reduces to

$${}^q\hat{\alpha}^i = {}^q\hat{\alpha}^i \Big|_{\text{ref}} + \sum_{j=1}^6 \frac{\partial({}^q\hat{\alpha}^i)}{\partial({}^{q\sigma}I^j)} \Big|_{\text{ref}} {}^{q\sigma}I^j + \frac{\partial({}^q\hat{\alpha}^i)}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 0, 1, \dots, 3 \quad (7.12)$$

By substituting from 7.12 into 7.10 we obtain the final form of the constitutive equation for the heat vector  $\bar{\mathbf{q}}^{(0)}$ . This is the most general form of the constitutive equation for the heat vector for thermofluids of order one.

## 7.2 Co-variant basis

In this case we have

$$[{}_d\bar{\sigma}_{(0)}] = [{}_d\bar{\sigma}_{(0)}](\bar{\rho}, [\gamma_{(1)}], \bar{\theta}, \bar{\mathbf{g}}) \quad (7.13)$$

$$\bar{\mathbf{q}}_{(0)} = \bar{\mathbf{q}}_{(0)}(\bar{\rho}, [\gamma_{(1)}], \bar{\theta}, \bar{\mathbf{g}}) \quad (7.14)$$

$$\bar{\Phi} = \bar{\Phi}(\bar{\rho}, \bar{\theta}) \quad (7.15)$$

We note that  $[\gamma^{(1)}] = [\gamma_{(1)}]$ , i.e., the first convected time derivative of the Almansi strain in contra-variant basis is the same as the first convected time derivative of Green's strain in the co-variant basis. Furthermore,  $\bar{\rho}$ ,  $\bar{\theta}$  and  $\bar{\mathbf{g}}$  are Eulerian descriptions involving coordinates  $\bar{x}_i$  of the material points in the current configuration and hence are independent of co- and contra-variant description. Hence, it is straight forward to conclude that  $[{}_d\bar{\sigma}_{(0)}] = [{}_d\bar{\sigma}^{(0)}]$  and  $\bar{\mathbf{q}}^{(0)} = \bar{\mathbf{q}}_{(0)}$ , i.e., for thermofluids of order one, the constitutive equations in the co- and contra-variant bases are identical.

### Remarks:

- (1) Since  $[\gamma^{(1)}] = [\gamma_{(1)}] = [D]$ , the symmetric part of the velocity gradient tensor in Eulerian description, its dyads are Cartesian, hence  $[{}_d\bar{\sigma}^{(0)}]$  and  $[{}_d\bar{\sigma}_{(0)}]$  for this case are tensors in the Cartesian  $x$ -frame. Thus, for this category of fluids, the distinction between co- and contra-variant measures disappears.
- (2) We generally define  $[{}_d\bar{\sigma}^{(0)}]$  and  $[{}_d\bar{\sigma}_{(0)}]$  as  $[{}_d\bar{\sigma}]$ , the Cauchy stress tensor whose dyads in this case are Cartesian in the fixed  $x$ -frame.
- (3) We emphasize again that the constitutive equations for the stress tensor for thermofluids of order one are indeed rate constitutive equations.
- (4) These constitutive equations hold for compressible thermoviscous fluids.

## 8 Constitutive equations for compressible generalized Newtonian and Newtonian fluids

### 8.1 Contra-variant basis: $[{}_d\bar{\sigma}^{(0)}]$ and $\bar{\mathbf{q}}^{(0)}$

If we consider contra-variant basis and if we assume that

$$[{}_d\bar{\sigma}^{(0)}] = [{}_d\bar{\sigma}^{(0)}](\bar{\rho}, [\gamma^{(1)}], \bar{\theta}) \quad (8.1)$$

$$\bar{\mathbf{q}}^{(0)} = \bar{\mathbf{q}}^{(0)}(\bar{\rho}, \bar{\theta}, \bar{\mathbf{g}}) \quad (8.2)$$

$$\bar{\Phi} = \bar{\Phi}(\bar{\rho}, \bar{\theta}) \quad (8.3)$$

then we can derive a much simplified form of the constitutive equations that describe simple thermoviscous fluids such as generalized Newtonian fluids and Newtonian fluids. We present details in the following.

### Deviatoric Cauchy stress $[_d\bar{\sigma}^{(0)}]$

In this case the generators are only due to  $[\gamma^{(1)}]$

$$[\sigma_{\sim} G^1] = [\gamma^{(1)}] \quad ; \quad [\sigma_{\sim} G^2] = [\gamma^{(1)}]^2 \quad (8.4)$$

$$\therefore \quad [_d\bar{\sigma}^{(0)}] = \sigma_{\sim} \tilde{\alpha}^0 [I] + \sigma_{\sim} \tilde{\alpha}^1 [\sigma_{\sim} G^1] + \sigma_{\sim} \tilde{\alpha}^2 [\sigma_{\sim} G^2] \quad (8.5)$$

The invariants are also only due to  $[\gamma^{(1)}]$

$$\sigma_{\sim} I^1 = \text{tr}([\gamma^{(1)}]) \quad ; \quad \sigma_{\sim} I^2 = \text{tr}([\gamma^{(1)}]^2) \quad ; \quad \sigma_{\sim} I^3 = \text{tr}([\gamma^{(1)}]^3) \quad (8.6)$$

Hence  $\sigma_{\sim} \tilde{\alpha}^i ; i = 0, 1, 2$  are functions of  $\bar{\rho}, \bar{\theta}$  and  $\sigma_{\sim} I^j ; j = 1, 2, 3$ . Consider Taylor series expansion of  $\sigma_{\sim} \tilde{\alpha}^i$  about the reference configuration and retain only up to the linear terms in the invariants and temperature.

$$\sigma_{\sim} \tilde{\alpha}^i = \sigma_{\sim} \tilde{\alpha}^i \Big|_{\text{ref}} + \sum_{j=1}^3 \frac{\partial(\sigma_{\sim} \tilde{\alpha}^i)}{\partial(\sigma_{\sim} I^j)} \Big|_{\text{ref}} (\sigma_{\sim} I^j - (\sigma_{\sim} I^j)_0) + \frac{\partial(\sigma_{\sim} \tilde{\alpha}^i)}{\partial \bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 0, 1, 2 \quad (8.7)$$

Since  $(\sigma_{\sim} I^j)_0 = 0 ; j = 1, 2, 3$  due to the fact that  $[\gamma^{(1)}]_0 = 0$ , expression 8.7 reduces to

$$\sigma_{\sim} \tilde{\alpha}^i = \sigma_{\sim} \tilde{\alpha}^i \Big|_{\text{ref}} + \sum_{j=1}^3 \frac{\partial(\sigma_{\sim} \tilde{\alpha}^i)}{\partial(\sigma_{\sim} I^j)} \Big|_{\text{ref}} \sigma_{\sim} I^j + \frac{\partial(\sigma_{\sim} \tilde{\alpha}^i)}{\partial \bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 0, 1, 2 \quad (8.8)$$

If we let  $\frac{\partial(\sigma_{\sim} \tilde{\alpha}^i)}{\partial(\sigma_{\sim} I^j)} = \sigma_{\sim} \tilde{\alpha}^i_{,j} ; j = 1, 2, 3$ , then 8.8 becomes

$$\sigma_{\sim} \tilde{\alpha}^i = \sigma_{\sim} \tilde{\alpha}^i \Big|_{\text{ref}} + \sum_{j=1}^3 (\sigma_{\sim} \tilde{\alpha}^i_{,j})_0 \sigma_{\sim} I^j + \frac{\partial(\sigma_{\sim} \tilde{\alpha}^i)}{\partial \bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 0, 1, 2 \quad (8.9)$$

Substitution from 8.6 into 8.9 and then from 8.9 into 8.5

$$\begin{aligned} [_d\bar{\sigma}^{(0)}] = & \left( \sigma_{\sim} \tilde{\alpha}^0 \Big|_{\text{ref}} + (\sigma_{\sim} \tilde{\alpha}^0_{,1})_0 \text{tr}([\gamma^{(1)}]) + (\sigma_{\sim} \tilde{\alpha}^0_{,2})_0 \text{tr}([\gamma^{(1)}]^2) + (\sigma_{\sim} \tilde{\alpha}^0_{,3})_0 \text{tr}([\gamma^{(1)}]^3) + \frac{\partial(\sigma_{\sim} \tilde{\alpha}^0)}{\partial \bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \right) [I] \\ & \left( \sigma_{\sim} \tilde{\alpha}^1 \Big|_{\text{ref}} + (\sigma_{\sim} \tilde{\alpha}^1_{,1})_0 \text{tr}([\gamma^{(1)}]) + (\sigma_{\sim} \tilde{\alpha}^1_{,2})_0 \text{tr}([\gamma^{(1)}]^2) + (\sigma_{\sim} \tilde{\alpha}^1_{,3})_0 \text{tr}([\gamma^{(1)}]^3) + \frac{\partial(\sigma_{\sim} \tilde{\alpha}^1)}{\partial \bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \right) [\gamma^{(1)}] \quad (8.10) \\ & \left( \sigma_{\sim} \tilde{\alpha}^2 \Big|_{\text{ref}} + (\sigma_{\sim} \tilde{\alpha}^2_{,1})_0 \text{tr}([\gamma^{(1)}]) + (\sigma_{\sim} \tilde{\alpha}^2_{,2})_0 \text{tr}([\gamma^{(1)}]^2) + (\sigma_{\sim} \tilde{\alpha}^2_{,3})_0 \text{tr}([\gamma^{(1)}]^3) + \frac{\partial(\sigma_{\sim} \tilde{\alpha}^2)}{\partial \bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \right) [\gamma^{(1)}]^2 \end{aligned}$$

Collecting coefficients and defining  $\tilde{\theta} = \bar{\theta} - \theta_0$ , then 8.10 can be written as

$$[_d\bar{\sigma}^{(0)}] = \sigma_{\sim} \tilde{\alpha}^0 \Big|_{\text{ref}} [I] + \frac{\partial(\sigma_{\sim} \tilde{\alpha}^0)}{\partial \bar{\theta}} \Big|_{\text{ref}} \tilde{\theta} [I] + \sigma_{\sim} b(\bar{\rho}, [\gamma^{(1)}], \bar{\theta}) [I] + \sigma_{\sim} b^1(\bar{\rho}, [\gamma^{(1)}], \bar{\theta}) [\gamma^{(1)}] + \sigma_{\sim} b^2(\bar{\rho}, [\gamma^{(1)}], \bar{\theta}) [\gamma^{(1)}]^2 \quad (8.11)$$

where

$$\begin{aligned} \sigma_{\sim} b(\bar{\rho}, [\gamma^{(1)}], \bar{\theta}) &= (\sigma_{\sim} \tilde{\alpha}^0_{,1})_0 \text{tr}([\gamma^{(1)}]) + (\sigma_{\sim} \tilde{\alpha}^0_{,2})_0 \text{tr}([\gamma^{(1)}]^2) + (\sigma_{\sim} \tilde{\alpha}^0_{,3})_0 \text{tr}([\gamma^{(1)}]^3) \\ \sigma_{\sim} b^1(\bar{\rho}, [\gamma^{(1)}], \bar{\theta}) &= \sigma_{\sim} \tilde{\alpha}^1 \Big|_{\text{ref}} + (\sigma_{\sim} \tilde{\alpha}^1_{,1})_0 \text{tr}([\gamma^{(1)}]) + (\sigma_{\sim} \tilde{\alpha}^1_{,2})_0 \text{tr}([\gamma^{(1)}]^2) + (\sigma_{\sim} \tilde{\alpha}^1_{,3})_0 \text{tr}([\gamma^{(1)}]^3) + \frac{\partial(\sigma_{\sim} \tilde{\alpha}^1)}{\partial \bar{\theta}} \Big|_{\text{ref}} \tilde{\theta} \quad (8.12) \\ \sigma_{\sim} b^2(\bar{\rho}, [\gamma^{(1)}], \bar{\theta}) &= \sigma_{\sim} \tilde{\alpha}^2 \Big|_{\text{ref}} + (\sigma_{\sim} \tilde{\alpha}^2_{,1})_0 \text{tr}([\gamma^{(1)}]) + (\sigma_{\sim} \tilde{\alpha}^2_{,2})_0 \text{tr}([\gamma^{(1)}]^2) + (\sigma_{\sim} \tilde{\alpha}^2_{,3})_0 \text{tr}([\gamma^{(1)}]^3) + \frac{\partial(\sigma_{\sim} \tilde{\alpha}^2)}{\partial \bar{\theta}} \Big|_{\text{ref}} \tilde{\theta} \end{aligned}$$

Equation 8.11 is the final form of the constitutive equations based on argument tensors in 8.1. This is the most general form of the constitutive equations for generalized Newtonian fluids. We note that 8.11 is quadratic in  $[\gamma^{(1)}]$ , i.e., it has generators  $[\gamma^{(1)}]$  and  $[\gamma^{(1)}]^2$ . The coefficients  $\sigma b$ ,  $\sigma b^1$  and  $\sigma b^2$  are functions of the invariants of the strain rate tensor  $[\gamma^{(1)}]$ , density  $\bar{\rho}$  and temperature  $\bar{\theta}$ . The first term on the right side of equation 8.11 describes the initial stress field in the reference configuration. The second term accounts for the stress field in the current configuration due to expansion and contraction.

In order to derive the constitutive equations similar to power law or Carreau-Yasuda models [4] for compressible thermoviscous fluids of order one, we simplify 8.11 by neglecting the generator  $[\gamma^{(1)}]^2$ , the invariant  $\text{tr}([\gamma^{(1)}]^3)$  and the last term in the expression for  $\sigma b^1$ .

$$[{}_d\bar{\sigma}^{(0)}] = \sigma \tilde{\alpha}^0 \Big|_{\text{ref}} \left[ I + \frac{\partial(\sigma \tilde{\alpha}^0)}{\partial \bar{\theta}} \right] \Big|_{\text{ref}} \tilde{\theta} [I] + \sigma b(\bar{\rho}, [\gamma^{(1)}], \bar{\theta}) [I] + \sigma b^1(\bar{\rho}, [\gamma^{(1)}], \bar{\theta}) [\gamma^{(1)}] \quad (8.13)$$

where

$$\begin{aligned} \sigma b(\bar{\rho}, [\gamma^{(1)}], \bar{\theta}) &= (\sigma \tilde{\alpha}^0, {}_1)_0 \text{tr}([\gamma^{(1)}]) + (\sigma \tilde{\alpha}^0, {}_2)_0 \text{tr}([\gamma^{(1)}]^2) \\ \sigma b^1(\bar{\rho}, [\gamma^{(1)}], \bar{\theta}) &= \sigma \tilde{\alpha}^1 \Big|_{\text{ref}} + (\sigma \tilde{\alpha}^1, {}_1)_0 \text{tr}([\gamma^{(1)}]) + (\sigma \tilde{\alpha}^1, {}_2)_0 \text{tr}([\gamma^{(1)}]^2) \end{aligned} \quad (8.14)$$

#### Further assumptions and simplifications:

If we assume that  $[{}_d\bar{\sigma}^{(0)}]$  only depends on the generator  $[\gamma^{(1)}]$ , then 8.11 reduces to

$$[{}_d\bar{\sigma}^{(0)}] = \sigma \tilde{\alpha}^0 \Big|_{\text{ref}} \left[ I + \frac{\partial(\sigma \tilde{\alpha}^0)}{\partial \bar{\theta}} \right] \Big|_{\text{ref}} \tilde{\theta} [I] + \sigma b(\bar{\rho}, [\gamma^{(1)}], \bar{\theta}) [I] + \sigma b^1(\bar{\rho}, [\gamma^{(1)}], \bar{\theta}) [\gamma^{(1)}] \quad (8.15)$$

in which the coefficients  $\sigma b$  and  $\sigma b^1$  remain the same as in 8.12. The constitutive equation 8.15 describes thermoviscous compressible generalized Newtonian fluids.

Equation 8.15 can be further simplified if we neglect the infinitesimals of orders two and higher in the velocity gradients appearing in  $[\gamma^{(1)}]$  and its invariants.

$$[{}_d\bar{\sigma}^{(0)}] = \sigma \tilde{\alpha}^0 \Big|_{\text{ref}} \left[ I + \frac{\partial(\sigma \tilde{\alpha}^0)}{\partial \bar{\theta}} \right] \Big|_{\text{ref}} \tilde{\theta} [I] + (\sigma \tilde{\alpha}^0, {}_1)_0 \text{tr}([\gamma^{(1)}]) [I] + \sigma \tilde{\alpha}^1 \Big|_{\text{ref}} [\gamma^{(1)}] \quad (8.16)$$

Let us define

$$\kappa(\bar{\rho}, \bar{\theta}) = (\sigma \tilde{\alpha}^0, {}_1)_0 \quad ; \quad 2\eta(\bar{\rho}, \bar{\theta}) = \sigma \tilde{\alpha}^1 \Big|_{\text{ref}} \quad (8.17)$$

Then 8.16 becomes

$$[{}_d\bar{\sigma}^{(0)}] = \sigma \tilde{\alpha}^0 \Big|_{\text{ref}} \left[ I + \frac{\partial(\sigma \tilde{\alpha}^0)}{\partial \bar{\theta}} \right] \Big|_{\text{ref}} \tilde{\theta} [I] + \kappa(\bar{\rho}, \bar{\theta}) \text{tr}([\gamma^{(1)}]) [I] + 2\eta(\bar{\rho}, \bar{\theta}) [\gamma^{(1)}] \quad (8.18)$$

This is the constitutive equation for thermoviscous compressible Newtonian fluids. If the reference configuration is stress free and if the stress field due to expansion and contraction are neglected then 8.18 reduces to

$$[{}_d\bar{\sigma}^{(0)}] = 2\eta(\bar{\rho}, \bar{\theta}) [\gamma^{(1)}] + \kappa(\bar{\rho}, \bar{\theta}) \text{tr}([\gamma^{(1)}]) [I] \quad (8.19)$$

which is the standard constitutive equation for compressible Newtonian fluids.  $\eta$  is Newtonian viscosity and  $\kappa$  is the second viscosity.

#### Heat vector $\bar{q}^{(0)}$

In this case the only generator is  $\bar{g}$ , hence we can write

$$\bar{q}^{(0)} = -^q \tilde{\alpha} \bar{g} \quad (8.20)$$

Also, in this case the only invariant is  $qI^1 = \bar{\mathbf{g}} \cdot \bar{\mathbf{g}}$ . Thus  $q\tilde{\alpha}$  is a function of  $\bar{\rho}$ ,  $\bar{\theta}$  and  $qI^1$  and  $\bar{\theta}$ . Expanding  $q\tilde{\alpha}$  in Taylor series about the reference configuration and retaining only up to linear terms in the invariant and temperature

$$q\tilde{\alpha} = q\tilde{\alpha}\Big|_{\text{ref}} + \frac{\partial(q\tilde{\alpha})}{\partial(qI^1)}\Big|_{\text{ref}} (qI^1 - (qI^1)_0) + \frac{\partial(q\tilde{\alpha})}{\partial\bar{\theta}}\Big|_{\text{ref}} (\bar{\theta} - \theta) \quad (8.21)$$

As before  $(qI^1)_0 = 0$ . Hence 8.21 reduces to

$$q\tilde{\alpha} = q\tilde{\alpha}\Big|_{\text{ref}} + \frac{\partial(q\tilde{\alpha})}{\partial(qI^1)}\Big|_{\text{ref}} qI^1 + \frac{\partial(q\tilde{\alpha})}{\partial\bar{\theta}}\Big|_{\text{ref}} (\bar{\theta} - \theta) \quad (8.22)$$

Substituting 8.22 into 8.20

$$\bar{\mathbf{q}}^{(0)} = -\left( q\tilde{\alpha}\Big|_{\text{ref}} + \frac{\partial(q\tilde{\alpha})}{\partial(qI^1)}\Big|_{\text{ref}} qI^1 + \frac{\partial(q\tilde{\alpha})}{\partial\bar{\theta}}\Big|_{\text{ref}} (\bar{\theta} - \theta) \right) \bar{\mathbf{g}} \quad (8.23)$$

which can be written as

$$\bar{\mathbf{q}}^{(0)} = -q\tilde{\alpha}\Big|_{\text{ref}} \bar{\mathbf{g}} - \frac{\partial(q\tilde{\alpha})}{\partial(qI^1)}\Big|_{\text{ref}} qI^1 \bar{\mathbf{g}} - \frac{\partial(q\tilde{\alpha})}{\partial\bar{\theta}}\Big|_{\text{ref}} (\bar{\theta} - \theta) \bar{\mathbf{g}} \quad (8.24)$$

Substituting for  $qI^1$  yields

$$\bar{\mathbf{q}}^{(0)} = -q\tilde{\alpha}\Big|_{\text{ref}} \bar{\mathbf{g}} - \frac{\partial(q\tilde{\alpha})}{\partial(qI^1)}\Big|_{\text{ref}} (\bar{\mathbf{g}} \cdot \bar{\mathbf{g}}) \bar{\mathbf{g}} - \frac{\partial(q\tilde{\alpha})}{\partial\bar{\theta}}\Big|_{\text{ref}} (\bar{\theta} - \theta) \bar{\mathbf{g}} \quad (8.25)$$

Equation 8.25 holds regardless whether the fluid is compressible or incompressible. This is the most general form of the constitutive relations for the heat vector with the assumed form for  $\bar{\mathbf{q}}^{(0)}$  in 8.20. If we neglect infinitesimals of order two and higher in the components of  $\bar{\mathbf{g}}$  and if we neglect the last term in 8.25, then 8.25 reduces to

$$\bar{\mathbf{q}}^{(0)} = -q\tilde{\alpha}\Big|_{\text{ref}} \bar{\mathbf{g}} \quad (8.26)$$

Let us define

$$k(\bar{\rho}, \bar{\theta}) = q\tilde{\alpha}\Big|_{\text{ref}} \quad (8.27)$$

Then 8.26 becomes

$$\bar{\mathbf{q}}^{(0)} = -k(\bar{\rho}, \bar{\theta}) \bar{\mathbf{g}} = -k(\bar{\rho}, \bar{\theta}) [I] \bar{\mathbf{g}} = -[K(\bar{\rho}, \bar{\theta})] \bar{\mathbf{g}} \quad (8.28)$$

in which  $k(\bar{\rho}, \bar{\theta})$  is thermal conductivity and  $[K(\bar{\rho}, \bar{\theta})]$  is the diagonal thermal conductivity matrix. 8.28 is the standard Fourier heat conduction law.

## 8.2 Co-variant basis: $[_d\bar{\sigma}_{(0)}]$ and $\bar{\mathbf{q}}_{(0)}$

Following details parallel to 8.1 in contra-variant basis, we consider the following in co-variant basis.

$$[_d\bar{\sigma}_{(0)}] = [_d\bar{\sigma}_{(0)}](\bar{\rho}, [\gamma_{(1)}], \bar{\theta}) \quad (8.29)$$

$$\bar{\mathbf{q}}_{(0)} = \bar{\mathbf{q}}_{(0)}(\bar{\rho}, \bar{\theta}, \bar{\mathbf{g}}) \quad (8.30)$$

$$\bar{\Phi} = \bar{\Phi}(\bar{\rho}, \bar{\theta}) \quad (8.31)$$

Here  $\bar{\rho}$ ,  $\bar{\theta}$  and  $\bar{\mathbf{g}}$  are independent of the choice of basis and  $[\gamma^{(1)}] = [\gamma_{(1)}]$ . Hence for this choice of argument tensors we have

$$[_d\bar{\sigma}_{(0)}] = [_d\bar{\sigma}^{(0)}] \quad (8.32)$$

and  $\bar{\mathbf{q}}_{(0)} = \bar{\mathbf{q}}^{(0)}$

Thus the derivations presented in sections 8.1 and 8.1 all hold for co-variant basis by replacing  $[\gamma^{(1)}]$  with  $[\gamma_{(1)}]$  (for the sake of clarity).

## 9 Incompressible thermoviscous ordered fluids

All of the derivations for  $[_d\bar{\sigma}^{(0)}]$ ,  $\bar{\mathbf{q}}^{(0)}$  and  $[_d\bar{\sigma}_{(0)}]$ ,  $\bar{\mathbf{q}}_{(0)}$  presented so far are for compressible fluids. In this section we consider incompressible ordered thermoviscous fluids. In case of incompressible matter

$$\text{div}(\mathbf{v}) = 0 \quad (9.1)$$

due to continuity equation which implies that

$$\text{tr}([\gamma^{(1)}]) = \text{tr}([\gamma_{(1)}]) = \text{tr}([\gamma^{(0)}]) = \text{tr}([\gamma_{(0)}]) = 0 \quad (9.2)$$

or alternatively, since  $\bar{\rho} = \rho = \text{constant}$ , then

$$\det[J] = 1 \quad (9.3)$$

must also hold for incompressible matter.

### 9.1 Argument tensors for Cauchy stress deviation, heat vector and $\bar{\Phi}$

**Contra-variant basis:**

$$\bar{\Phi} = \bar{\Phi}(\bar{\theta}(\bar{\mathbf{x}}, t)) \quad (9.4)$$

$$[\bar{\sigma}^{(0)}] = [\bar{\sigma}^{(0)}([\gamma^{(j)}(\bar{\mathbf{x}}, t)]; j = 1, 2, \dots, n, \bar{\theta}(\bar{\mathbf{x}}, t), \bar{\mathbf{g}}(\bar{\mathbf{x}}, t))] \quad (9.5)$$

$$[\bar{\sigma}^{(0)}] = [_e\bar{\sigma}^{(0)}] + [_d\bar{\sigma}^{(0)}([\gamma^{(j)}(\bar{\mathbf{x}}, t)]; j = 1, 2, \dots, n, \bar{\theta}(\bar{\mathbf{x}}, t), \bar{\mathbf{g}}(\bar{\mathbf{x}}, t))] \quad (9.6)$$

$$\bar{\mathbf{q}}^{(0)} = \bar{\mathbf{q}}^{(0)}([\gamma^{(j)}(\bar{\mathbf{x}}, t)]; j = 1, 2, \dots, n, \bar{\theta}(\bar{\mathbf{x}}, t), \bar{\mathbf{g}}(\bar{\mathbf{x}}, t)) \quad (9.7)$$

$$[_e\bar{\sigma}^{(0)}] = p(\bar{\theta})[I] \quad (9.8)$$

**Co-variant basis:**

$$\bar{\Phi} = \bar{\Phi}(\bar{\theta}(\bar{\mathbf{x}}, t)) \quad (9.9)$$

$$[\bar{\sigma}_{(0)}] = [\bar{\sigma}_{(0)}([\gamma_{(j)}(\bar{\mathbf{x}}, t)]; j = 1, 2, \dots, n, \bar{\theta}(\bar{\mathbf{x}}, t), \bar{\mathbf{g}}(\bar{\mathbf{x}}, t))] \quad (9.10)$$

$$[\bar{\sigma}_{(0)}] = [_e\bar{\sigma}_{(0)}] + [_d\bar{\sigma}_{(0)}([\gamma_{(j)}(\bar{\mathbf{x}}, t)]; j = 1, 2, \dots, n, \bar{\theta}(\bar{\mathbf{x}}, t), \bar{\mathbf{g}}(\bar{\mathbf{x}}, t))] \quad (9.11)$$

$$\bar{\mathbf{q}}_{(0)} = \bar{\mathbf{q}}_{(0)}([\gamma_{(j)}(\bar{\mathbf{x}}, t)]; j = 1, 2, \dots, n, \bar{\theta}(\bar{\mathbf{x}}, t), \bar{\mathbf{g}}(\bar{\mathbf{x}}, t)) \quad (9.12)$$

$$[_e\bar{\sigma}_{(0)}] = p(\bar{\theta})[I] \quad (9.13)$$

### 9.2 Most general form of the constitutive equations

The general theory presented in section 3 and the constitutive equations for thermofluids of order one presented in section 7 can be easily modified by incorporating the incompressibility assumptions 9.1 - 9.3. This is straight forward and hence the details are omitted. The constitutive equations presented in section 8 for compressible generalized Newtonian fluids and Newtonian fluids are used to derive the constitutive equations for the incompressible case in the following sections.

### 9.3 Constitutive equations for incompressible generalized Newtonian and Newtonian fluids

In this case 8.1 - 8.3 reduce to (using contra-variant basis)

$$[_d\bar{\sigma}^{(0)}] = [_d\bar{\sigma}^{(0)}([\gamma^{(1)}], \bar{\theta})] \quad (9.14)$$

$$\bar{\mathbf{q}}^{(0)} = \bar{\mathbf{q}}^{(0)}(\bar{\theta}, \bar{\mathbf{g}}) \quad (9.15)$$

$$\bar{\Phi} = \bar{\Phi}(\bar{\theta}) \quad (9.16)$$

and the incompressibility assumptions yield

$$\sigma \tilde{I}^1 = \text{tr}([\gamma^{(1)}]) = 0 \quad (9.17)$$

Hence, following the derivation in section 8.1, we can obtain 8.11 in which the coefficients  $\sigma b$ ,  $\sigma b^1$  and  $\sigma b^2$  must be modified using 9.17. If we assume that  $[_d\bar{\sigma}^{(0)}]$  only depends on the generator  $[\gamma^{(1)}]$ , then 8.11 reduces to 8.15 in which  $\sigma b$  and  $\sigma b^1$  are modified to account for incompressibility. We present details in the following. In this case we have

$$[_d\bar{\sigma}^{(0)}] = \sigma \tilde{\alpha}^0 \Big|_{\text{ref}} [I] + \frac{\partial(\sigma \tilde{\alpha}^0)}{\partial \bar{\theta}} \Big|_{\text{ref}} \tilde{\theta} [I] + \sigma b([\gamma^{(1)}], \bar{\theta}) [I] + \sigma b^1([\gamma^{(1)}], \bar{\theta}) [\gamma^{(1)}] \quad (9.18)$$

in which

$$\begin{aligned} \sigma b([\gamma^{(1)}], \bar{\theta}) &= (\sigma \tilde{\alpha}^0, 2)_0 \text{tr}([\gamma^{(1)}]^2) + (\sigma \tilde{\alpha}^0, 3)_0 \text{tr}([\gamma^{(1)}]^3) \\ \sigma b^1([\gamma^{(1)}], \bar{\theta}) &= \sigma \tilde{\alpha}^1 \Big|_{\text{ref}} + (\sigma \tilde{\alpha}^1, 2)_0 \text{tr}([\gamma^{(1)}]^2) + (\sigma \tilde{\alpha}^1, 3)_0 \text{tr}([\gamma^{(1)}]^3) + \frac{\partial(\sigma \tilde{\alpha}^1)}{\partial \bar{\theta}} \Big|_{\text{ref}} \tilde{\theta} \end{aligned} \quad (9.19)$$

These describe the most general form of thermoviscous incompressible generalized Newtonian fluids based in 9.14 - 9.17.

If we neglect infinitesimals of order three in the components of  $[\gamma^{(1)}]$ , then we can neglect the terms containing  $\text{tr}([\gamma^{(1)}]^3)$  in 9.19 which results in modification of the coefficients  $\sigma b$ ,  $\sigma b^1$  and

$$\begin{aligned} \sigma b([\gamma^{(1)}], \bar{\theta}) &= (\sigma \tilde{\alpha}^0, 2)_0 \text{tr}([\gamma^{(1)}]^2) \\ \sigma b^1([\gamma^{(1)}], \bar{\theta}) &= \sigma \tilde{\alpha}^1 \Big|_{\text{ref}} + (\sigma \tilde{\alpha}^1, 2)_0 \text{tr}([\gamma^{(1)}]^2) + \frac{\partial(\sigma \tilde{\alpha}^1)}{\partial \bar{\theta}} \Big|_{\text{ref}} \tilde{\theta} \end{aligned} \quad (9.20)$$

Substituting 9.20 into 9.18

$$\begin{aligned} [_d\bar{\sigma}^{(0)}] &= \sigma \tilde{\alpha}^0 \Big|_{\text{ref}} [I] + \frac{\partial(\sigma \tilde{\alpha}^0)}{\partial \bar{\theta}} \Big|_{\text{ref}} \tilde{\theta} [I] + (\sigma \tilde{\alpha}^0, 2)_0 \text{tr}([\gamma^{(1)}]^2) [I] \\ &\quad + \left( \sigma \tilde{\alpha}^1 \Big|_{\text{ref}} + (\sigma \tilde{\alpha}^1, 2)_0 \text{tr}([\gamma^{(1)}]^2) + \frac{\partial(\sigma \tilde{\alpha}^1)}{\partial \bar{\theta}} \Big|_{\text{ref}} \tilde{\theta} \right) [\gamma^{(1)}] \end{aligned} \quad (9.21)$$

which can be written as

$$\begin{aligned} [_d\bar{\sigma}^{(0)}] &= \sigma \tilde{\alpha}^0 \Big|_{\text{ref}} [I] + \frac{\partial(\sigma \tilde{\alpha}^0)}{\partial \bar{\theta}} \Big|_{\text{ref}} \tilde{\theta} [I] + \sigma \tilde{\alpha}^1 \Big|_{\text{ref}} [\gamma^{(1)}] + (\sigma \tilde{\alpha}^0, 2)_0 \text{tr}([\gamma^{(1)}]^2) [I] \\ &\quad + \left( (\sigma \tilde{\alpha}^1, 2)_0 \text{tr}([\gamma^{(1)}]^2) + \frac{\partial(\sigma \tilde{\alpha}^1)}{\partial \bar{\theta}} \Big|_{\text{ref}} \tilde{\theta} \right) [\gamma^{(1)}] \end{aligned} \quad (9.22)$$

Equation 9.22 is the simplified form of the thermoviscous incompressible generalized Newtonian fluid. If we define

$$\begin{aligned} 2\eta(\bar{\theta}) &= \sigma \tilde{\alpha}^1 \Big|_{\text{ref}} \\ \eta_1(\text{tr}([\gamma^{(1)}]^2), \bar{\theta}) &= (\sigma \tilde{\alpha}^0, 2)_0 \text{tr}([\gamma^{(1)}]^2) \\ \eta_2(\text{tr}([\gamma^{(1)}]^2), \bar{\theta}) &= (\sigma \tilde{\alpha}^1, 2)_0 \text{tr}([\gamma^{(1)}]^2) + \frac{\partial(\sigma \tilde{\alpha}^1)}{\partial \bar{\theta}} \Big|_{\text{ref}} \tilde{\theta} \end{aligned} \quad (9.23)$$

Thus 9.22 can be written as

$$[_d\bar{\sigma}^{(0)}] = \sigma \tilde{\alpha}^0 \Big|_{\text{ref}} [I] + \frac{\partial(\sigma \tilde{\alpha}^0)}{\partial \bar{\theta}} \Big|_{\text{ref}} \tilde{\theta} [I] + 2\eta(\bar{\theta}) [\gamma^{(1)}] + \eta_1(\text{tr}([\gamma^{(1)}]^2), \bar{\theta}) [I] + \eta_2(\text{tr}([\gamma^{(1)}]^2), \bar{\theta}) [\gamma^{(1)}] \quad (9.24)$$

where  $\eta$  is Newtonian viscosity dependent on the temperature  $\bar{\theta}$  in the current configuration.  $\eta_1$  and  $\eta_2$  are coefficients dependent on the second invariant of  $[\gamma^{(1)}]$  and the temperature  $\bar{\theta}$  in the current configuration. At this point we remark that none of the constitutive equations for  $[_d\bar{\sigma}^{(0)}]$  presented here for generalized Newtonian fluids compare with either power law or Carreau-Yasuda models that are commonly used. In 9.24 if we neglect infinitesimals of order two of the components of  $[\gamma^{(1)}]$ , i.e., neglect  $\text{tr}([\gamma^{(1)}]^2)$  terms, and the last term in the expression for  $\eta_2$  then 9.24 reduces to

$$[_d\bar{\sigma}^{(0)}] = \sigma \tilde{\alpha}^0 \Big|_{\text{ref}} [I] + \frac{\partial(\sigma \tilde{\alpha}^0)}{\partial \theta} \Big|_{\text{ref}} \tilde{\theta}[I] + 2\eta(\bar{\theta})[\gamma^{(1)}] \quad (9.25)$$

The constitutive equations 9.25 describe thermoviscous incompressible Newtonian fluids in which  $\eta(\bar{\theta})$  is temperature dependent viscosity.

The constitutive equation for the heat vector  $\bar{\mathbf{q}}^{(0)}$  follows the same procedure as for compressible case except that we need some modifications to account for incompressibility, i.e.,  $\bar{\rho} = \rho = \text{constant}$  and  $\text{tr}([\gamma^{(1)}]) = 0$ . Details are straight forward and hence are omitted.

**Remarks:**

- (1) The constitutive equations in co-variant basis can be easily obtained by replacing  $[\gamma^{(i)}]$  with  $[\gamma_{(i)}]$ ;  $i = 1, 2, \dots, n$  in the derivations presented for the contra-variant basis.
- (2) From the derivations presented here for generalized Newtonian fluids we note that Power law and Carreau-Yasuda models [3, 4] for generalized Newtonian fluids are not derivable from the constitutive theory.
- (3) Temperature dependent viscosity, i.e.,  $\eta(\bar{\theta})$  and also  $\eta_1(\bar{\theta})$ ,  $\eta_2(\bar{\theta})$  are valid. Thus Sutherland's law and power law for temperature dependent viscosity are valid as long as the viscosity is positive so that the requirement of positive viscous dissipation (due to entropy inequality) is not violated.

## 10 Summary and conclusions

We have presented development of rate constitutive theory for incompressible as well as compressible ordered thermofluids in contra-variant and co-variant bases. Based on the axiom of admissibility, all constitutive theory must satisfy conservation laws to ensure thermodynamic equilibrium of the deforming matter. Since conservation of mass, balance of momenta and energy equation only require existence of the stress field and heat vector, these are independent of the constitution of the matter. Thus the second law of thermodynamics (Clausius-Duhem inequality) must provide the basis for the constitutive theory.

The conditions resulting from the Clausius-Duhem inequality: (i) Show that  $\eta$ , specific entropy is deterministic from the Helmholtz free energy and hence should not be considered as a dependent variable in the constitutive theory. Thus, the stress tensor, heat vector and the Helmholtz free energy density are the only dependent variables in the constitutive theory for the type of fluids considered here. (ii) Provide a mechanism to determine the heat vector as a function of the temperature gradient vector and conductivity, i.e., Fourier heat condition law (iii) Do not provide a mechanism to determine constitutive equations for the total stress tensor. However, if the total Cauchy stress tensor is decomposed into equilibrium stress and deviatoric stress, then: (a) The equilibrium stress is deterministic from the entropy inequality and leads to thermodynamic pressure for compressible fluids and mechanical pressure in the case of incompressible fluids. The derivations are presented in this chapter. These hold regardless of the order of the thermofluid. (b) But the deviatoric stress is not deterministic from the entropy inequality, however the entropy inequality does require the dissipation due to the deviatoric Cauchy stress to be positive. Thus the constitutive theory for ordered thermofluids reduces to deviatoric Cauchy stress tensor, heat vector and Helmholtz free energy density as dependent variables and their determination in terms of the argument tensors describing the flow physics in contra-variant and co-variant bases.

Details of the contra- and co-variant bases, stress and strain measures, convected time derivatives of the stress and strain tensors in contra- and co-variant bases, derivations of entropy inequality and the conditions resulting from it are presented in this chapter. It is shown that for compressible ordered thermofluids: (i) in

contra-variant basis, the argument tensors of deviatoric stress  $[_d\bar{\sigma}^{(0)}]$  and heat vector  $\bar{\mathbf{q}}^{(0)}$  are  $\bar{\rho}$ ,  $\bar{\theta}$ ,  $\bar{\mathbf{g}}$  and  $[\gamma^{(j)}]$ ;  $j = 1, 2, \dots, n$  the convected time derivatives of orders  $1, 2, \dots, n$  in the contra-variant basis and for  $\bar{\Phi}$ , the argument tensors are  $\bar{\rho}$  and  $\bar{\theta}$ . (ii) in co-variant basis, the argument tensors of the deviatoric stress  $[_d\bar{\sigma}_{(0)}]$  and heat vector  $\bar{\mathbf{q}}_{(0)}$  are  $\bar{\rho}$ ,  $\bar{\theta}$ ,  $\bar{\mathbf{g}}$  and  $[\gamma_{(j)}]$ ;  $j = 1, 2, \dots, n$  the convected time derivatives of orders  $1, 2, \dots, n$  in the co-variant basis and for  $\bar{\Phi}$ , the argument tensors are  $\bar{\rho}$  and  $\bar{\theta}$ . For incompressible ordered thermofluids, density  $\bar{\rho}$  in the current configuration is the same as in the reference configuration and hence it is no longer an argument of the dependent variables in the constitutive theory. Other arguments remain the same as for the compressible case.

The theory of generators and invariants is utilized to derive the general form of the constitutive theory for an  $n^{th}$  order ‘ordered thermofluid’ (both compressible and incompressible) in contra-variant and co-variant bases. In this theory both the deviatoric Cauchy stress and the heat vectors are expressed as a linear combination of the combined generators of the argument tensors. The coefficients in this linear combination are functions of the combined invariants of the argument tensors in addition to  $\bar{\rho}$  and  $\bar{\theta}$  (in case of compressible fluids) or  $\bar{\theta}$  (in case of incompressible fluids). The coefficients are determined by using their Taylor series expansion about the reference configuration and retaining only up to linear terms in the combined invariants and temperature. Explicit details are presented for second order ‘ordered thermofluids’.

The general form of the constitutive equations are specialized and detailed derivations are presented for thermoviscous generalized Newtonian and Newtonian fluids (both compressible and incompressible). For such fluids, only the first convected time derivative of the strain tensor (Green or Almansi depending upon co- or contra-variant basis) remains as argument tensor for the deviatoric stress (in addition to density and temperature). The heat vector does not contain the first convected time derivative of the strain tensor as an argument.

Based on the theory presented in this chapter for ordered thermofluids we make the following specific remarks and draw some conclusions.

1. For ordered thermofluids of order greater than or equal to two (i.e., when  $[\gamma^{(2)}]$ ,  $[\gamma^{(3)}]$ ,  $\dots$  or  $[\gamma_{(2)}]$ ,  $[\gamma_{(3)}]$ ,  $\dots$  are argument tensors), the contra- and co-variant stress measures are not the same, i.e., in this case  $[_d\bar{\sigma}^{(0)}] \neq [_d\bar{\sigma}_{(0)}]$ . Thus, their dyads and magnitudes associated with the dyads are different. Hence, in such cases the co- and contra-variant measures must be transformed to Cartesian basis ( $x$ -frame) using  $[J]$  and/or  $[\bar{J}]$  before using them in the momentum and energy equations if the deformation is finite.
2. For ordered thermofluids of order one, i.e., when  $[\gamma^{(1)}]$  or  $[\gamma_{(1)}]$  are argument tensors, the contra- and co-variant stress measures are the same, i.e., in this case  $[_d\bar{\sigma}^{(0)}] = [_d\bar{\sigma}_{(0)}]$  and are indeed in the  $x$ -frame. This can be verified by the dyads on the right side of the stress tensor equation. For such fluids, the distinction between contra- and co-variant bases disappears and we may simply say deviatoric Cauchy stress  $[_d\bar{\sigma}]$  as opposed to contra- and co-variant deviatoric Cauchy stress tensor which in fact is the tensor in the  $x$ -frame. Thus, for generalized Newtonian and Newtonian fluids (both compressible and incompressible) the co-variant and contra-variant stress measures are the same and are in fact in the  $x$ -frame and hence, their use in momentum and energy equation (in  $x$ -frame) is valid. We note that these constitutive relations are not valid for finite deformation.
3. Based on the theory of generators and invariants, the constitutive theory for heat vector for an ordered thermofluid is much more complex (even for thermofluids of order one due to the dependence of the heat vector on the combined generators of  $[\gamma^{(1)}]$ ,  $\bar{\mathbf{g}}$  or  $[\gamma_{(1)}]$ ,  $\bar{\mathbf{g}}$ ) compared to Fourier heat conduction law which requires that the heat vector not be dependent on  $[\gamma^{(1)}]$  or  $[\gamma_{(1)}]$ . The constitutive theory for the heat vector based on the combined generators of  $[\gamma^{(1)}]$ ,  $\bar{\mathbf{g}}$  or  $[\gamma_{(1)}]$ ,  $\bar{\mathbf{g}}$  is perhaps more realistic for fluids as it accounts for velocity gradients. However, their use will require experimental determination of additional constants or coefficients.
4. From the general and specific derivations presented for generalized Newtonian fluids, it is clear that power law and Carreau-Yasuda constitutive models [2–4] used currently are not derivable using continuum mechanics theory of constitutive equations. The derivations presented here clearly show dependence of the medium viscosity on the second invariant of the first convected time derivative of the strain tensor but not in the same manner as it appears in power law and Carreau-Yasuda models.
5. A significant point to note is that all constitutive theory for ordered thermofluids in contra- or co-variant bases are in fact rate constitutive theories. In the case of constitutive equations in the contra-variant

basis, we express the convected time derivative of order zero of the contra-variant deviatoric Cauchy stress tensor  $[\bar{\sigma}^{(0)}]$  in terms of the convected time derivatives of various orders of the Almansi strain tensor in the contra-variant basis. Likewise, for the constitutive equations in the co-variant basis, we express the convected time derivative of order zero of the co-variant deviatoric Cauchy stress tensor  $[\bar{\sigma}_{(0)}]$  in terms of the convected time derivatives of various orders of the Green's strain tensor in the co-variant basis.

Thus, the constitutive equation for generalized Newtonian and Newtonian fluid are indeed rate constitutive equations. The distinction between co- and contra-variant measures disappears for such fluids due to the fact that the convected time derivative of order one of the Green's strain is the same as the convected time derivative of order one of the Almansi strain with the additional restriction of infinitesimal deformation.

6. It is significant to note that based on Surana et al. [13], when the deformation is finite, only the constitutive equations derived using contra-variant basis remain valid. As the magnitude of the deformation increases, the constitutive equations in co-variant basis and others become progressively more spurious.
7. The condition of positive dissipation resulting from the entropy inequality is satisfied by all rate constitutive equations presented here provided we observe certain restrictions on the coefficients such as the viscosity must be positive etc.
8. Since the constitutive theory in this chapter is based on combined generators and invariants of the argument tensors of the dependent variable, strictly speaking it lacks thermodynamic basis (as these are not derived using entropy inequality). However, the theory does have continuum mechanics foundation and it does satisfy the conditions resulting from entropy inequality.

The work presented in this chapter provides a completely general and unified theory for ordered thermofluids from which specialized fluid behaviors such as generalized Newtonian fluids, Newtonian fluids etc. can be easily derived. It is demonstrated that the distinction between contra- and co-variant bases is critical for ordered thermofluids of order greater than or equal to two.

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## Chapter 3

# Rate Constitutive Theory for Ordered Thermoelastic Solids

When the mathematical models for the deforming solids are constructed in Eulerian description, the material particle displacements and the strain measures are not readily obtainable. In such cases the constitutive theory must utilize convected time derivatives of the strain measures. This chapter presents development of rate constitutive theory for compressible as well as incompressible ordered thermoelastic homogeneous isotropic solids in contra- and co-variant bases. The density, temperature and temperature gradient in the current configuration and the convected time derivatives of the strain tensor up to any desired order are considered as the arguments of the first convected time derivative of the deviatoric Cauchy stress tensor, heat flux and the Helmholtz free energy density. The thermoelastic solids described by this constitutive theory are termed ordered thermoelastic solids due to the fact that the constitutive equations for the deviatoric Cauchy stress tensor and heat vector are dependent on the convected time derivatives of the strain tensor up to any desired order, the highest order defining the order of the solid.

As shown in reference [1] for ordered thermofluids, in this case also, the entropy inequality that forms the basis for constitutive theory only provides a mechanism for determining constitutive equations for the equilibrium stress with the additional requirement that energy dissipation due to the deviatoric part of the Cauchy stress be positive, but provides no mechanism for establishing constitutive equations for it.

It is shown that in the development of the constitutive theory one must consider a coordinate system in the current configuration in which the deformed material lines can be identified. Thus the co-variant and contra-variant convected coordinate systems are natural choices for the development of the constitutive theory. The compatible conjugate pairs of convected time derivatives of the stress and strain measures in conjunction with the theory of generators and invariants provide a general mathematical framework for the development of the constitutive theory for ordered thermoelastic solids. This framework has a foundation based on the basic principles and axioms of continuum mechanics and satisfies the condition of positive dissipation, a requirement resulting from the entropy inequality. In this chapter we present a general theory of rate constitutive equations for ordered thermoelastic solids which is then specialized assuming first order theory to obtain the commonly used constitutive equations for incompressible and compressible elastic solids.

The research work presented in this chapter is being submitted for a journal publication [2].

## 1 Introduction

The rate constitutive equations are generally derived using constitutive theory in which the stress rates are functions of the strain rates [3–6]. The need for such constitutive theory arises when the mathematical models for the deforming solid are constructed using Eulerian description in which material particles are not followed during the deformation. Therefore strain measures cannot be used in the development of the constitutive theory. Secondly, the most natural way to derive a constitutive theory (for homogeneous and isotropic matter) is to consider deformed material lines at a material point in the current configuration that correspond to the same material point in the reference configuration with orthogonal material lines. The deformed material lines in the

current configuration are curvilinear. The tangent vectors to these material lines at the material point constitute a non-orthogonal basis called co-variant basis. If we consider an elementary tetrahedron at a material point in the reference configuration with orthogonal material lines forming its edges, then upon deformation the co-variant vectors are indeed the edges of the deformed tetrahedron. Using the faces of the deformed tetrahedron that are formed by the pairs of co-variant base vectors, we can also define a reciprocal coordinate system called contra-variant coordinate system. The vectors forming this coordinate system are called contra-variant base vectors. The contra-variant base vectors are normal to the faces of the deformed tetrahedron. The co- and contra-variant bases are obviously related. Thus, in the deformed configuration, we have at least two possible bases, contra- and co-variant in which we could consider the development of the constitutive theory. As pointed out, the strain measures in these two bases are of no use in this constitutive theory under consideration as these require material particle displacement gradients. Thus we must consider the time derivatives of the strain measures in the co- and contra-variant bases and the time derivatives of the conjugate stress measures in the co- and contra-variant bases in the development of the constitutive theory. The resulting constitutive theory is the rate constitutive theory. Thus, it is clear that in the development of the rate constitutive theory, we must distinguish between co- and contra-variant bases and must consider both bases.

If we consider Green's strain [3–6] as a measure of finite strain in the co-variant basis, then we can obtain its time derivatives of various orders in the co-variant basis. These are called convected time derivatives of the Green's strain tensor. Similarly if we consider Almansi strain as a measure of finite strain in the contra-variant basis, then we can also obtain its time derivatives of various orders in the contra-variant basis. These are called convected time derivatives of the Almansi strain tensor. One could show that the convected time derivatives of all orders of the strain measures in both bases are objective, a strict requirement for them to be admissible in the constitutive theory.

Since we have co- and contra-variant bases in the deformed configuration and the convected time derivatives of the strain tensors, we must also define conjugate stress measures and their convected time derivatives in the two bases. For this purpose we define contra-variant Cauchy stress tensor and co-variant Cauchy stress tensor and their convected time derivatives of various orders in the respective bases. These are objective as well. In the rate constitutive theory we determine the relations that define the first convected time derivative of a chosen stress measure as a function of the convected time derivatives of the conjugate strain measures (and other arguments).

The concepts of convected time derivatives, the objective rates of the stress and strain tensors and their use in the constitutive models can be traced back to Jaumann (1905), Oldroyd B (1958), Giesekus (1962) in references [7–9] in connection with solid matter as well as polymeric liquids. Hypo-elasticity material laws [10–14] are a special form of the rate constitutive equations for linear elastic solid matter. Upper convected, lower convected, Jaumann rate constitutive equations have been used commonly in a large volume of published work on mathematical models and numerical computations [15–17] for solid matter. In many of these works the emphasis is on the use of the constitute models as opposed to their origin and the details of their derivations. The concept of 'ordered' seems to have been introduced in reference [5] in connection with fluids and used more recently by authors [1] in connection with thermofluids to derive a general rate constitutive theory for ordered thermofluids.

## Scope of present work

The work presented in this chapter focuses on the development of general theory of rate constitutive equations for ordered thermoelastic solids for which the mathematical models are in Eulerian description. In this constitutive theory, the first convected time derivative of the deviatoric Cauchy stress tensor and the heat vectors are expressed as functions of the convected time derivatives up to any desired order of the conjugate strain tensor, density  $\bar{\rho}$ , temperature  $\bar{\theta}$  and temperature gradient  $\bar{\mathbf{g}}$ . We begin all developments by using entropy inequality, an essential conservation law for the development of the constitutive theory. The Cauchy stress tensor is decomposed into equilibrium stress and deviatoric stress. This is necessitated due to the entropy inequality. The equilibrium stress for both compressible and incompressible cases is established using entropy inequality [1]. For the deviatoric Cauchy stress the entropy inequality does not provide any mechanism for establishing the constitutive theory. In the present work we use the theory of generators and invariants to: (i) establish a most general form of the rate constitutive equations in which the first convected time derivative of the chosen deviatoric Cauchy stress tensor can be a function of the convected time derivatives up to any desired order of

the conjugate strain tensor (and other arguments); (ii) specialize the general theory presented in (i) to second order thermoelastic solids; (iii) further specialize the theory presented in (ii) to first order thermoelastic solids and demonstrate that the general constitutive theory of ordered thermoelastic solids of order one reduces to the well known hypo-elasticity with further assumptions. All derivations and details in (i) - (iii) are presented using contra-variant as well as co-variant bases for incompressible and compressible cases. Using the derivations in these two bases, it is shown that Jaumann rate constitutive equations are easily derivable. Detailed discussion and arguments are presented to discuss the validity of the contra-variant and co-variant rate constitutive equations as well as the validity of Jaumann rate constitutive equations.

## 2 Preliminary material

### 2.1 Notation

In this section we present a very condensed brief account of coordinate systems, measures of stresses, strain and their convected time derivatives of various orders and helpful definitions that have been covered in details by the authors in reference [1] but presented here for convenience. Let  $x_i$  and  $\bar{x}_i$  denote position coordinates of a material point in the reference and current configurations in a fixed frame ( $x$ -frame). Then

$$\bar{x}_i = \bar{x}_i(x_1, x_2, x_3, t) \quad (2.1)$$

$$\text{or} \quad x_i = x_i(\bar{x}_1, \bar{x}_2, \bar{x}_3, t) \quad (2.2)$$

If  $\{dx\} = [dx_1, dx_2, dx_3]^t$  and  $\{d\bar{x}\} = [d\bar{x}_1, d\bar{x}_2, d\bar{x}_3]^t$  are the components of length  $ds$  and  $d\bar{s}$  in the reference and current configuration, and if we neglect the infinitesimals of orders two and higher in both configurations, then we can obtain the following [10]

$$\{d\bar{x}\} = [J]\{dx\} \quad (2.3)$$

$$\{dx\} = [\bar{J}]\{d\bar{x}\} \quad (2.4)$$

with

$$[J] = [\bar{J}]^{-1} \quad ; \quad [\bar{J}] = [J]^{-1} \quad ; \quad [J][\bar{J}] = [\bar{J}][J] = [I] \quad (2.5)$$

Using Murnaghan's notation

$$[J] = \frac{\partial\{\bar{x}\}}{\partial\{x\}} = \begin{bmatrix} \bar{x}_1 & \bar{x}_2 & \bar{x}_3 \\ x_1 & x_2 & x_3 \end{bmatrix} \quad ; \quad [\bar{J}] = \frac{\partial\{x\}}{\partial\{\bar{x}\}} = \begin{bmatrix} x_1 & x_2 & x_3 \\ \bar{x}_1 & \bar{x}_2 & \bar{x}_3 \end{bmatrix} \quad (2.6)$$

The columns of  $[J]$  are co-variant base vectors  $\tilde{\mathbf{g}}_i$  whereas the rows of  $[\bar{J}]$  are contra-variant base vectors  $\tilde{\mathbf{g}}^i$ .  $[J]$  and  $[\bar{J}]$  are Jacobians of deformation. That is, the basis of  $[\bar{J}]$  is reciprocal of the basis of  $[J]$ .

Few more useful relations [1] are given in the following:

$$\frac{D}{Dt}[J] = [L][J] \quad (2.7)$$

$$\frac{D}{Dt}[\bar{J}] = -[\bar{J}][L] \quad (2.8)$$

$$\text{where} \quad [L] = \frac{\partial v_i}{\partial \bar{x}_j} \mathbf{e}_i \mathbf{e}_j \quad (2.9)$$

in which  $\frac{D}{Dt}$  stands for the material derivative and  $v_i$  are velocity components in the  $x$ -frame.

### 2.2 Strain measures

In the present work we consider Green's strain  $[\varepsilon]$ , in co-variant basis, and Almansi strain  $[\bar{\varepsilon}]$ , in contra-variant basis, both being measures of finite strain [1]

$$[\varepsilon] = \frac{1}{2}([J]^t[J] - [I]) \quad (\text{Def.}) \quad (2.10)$$

$$[\bar{\varepsilon}] = \frac{1}{2}([I] - [\bar{J}][\bar{J}]^t) \quad (\text{Def.}) \quad (2.11)$$

Both  $[\varepsilon]$  and  $[\bar{\varepsilon}]$  contain Cartesian components.

### 2.3 Stress measures

Let  $[\bar{T}^{(0)}]$  be the Cauchy stress tensor in contra-variant basis that corresponds to the directions normal to the faces of the deformed tetrahedron in the current configuration [1]. Let  $[\bar{T}_{(0)}]$  be the Cauchy stress tensor in the co-variant basis. These correspond to a new tetrahedron such that co-variant base vectors are normal to its faces. We can obtain the Cartesian components of  $[\bar{T}^{(0)}]$  and  $[\bar{T}_{(0)}]$ . For compressible medium these are

$$[T] = [T]^t = |J|[\bar{J}][\bar{T}^{(0)}][\bar{J}]^t = [T^{[0]}] \quad (\text{Def.}) \quad (2.12)$$

$$[T] = [T]^t = |J|[\bar{J}]^t[\bar{T}_{(0)}][\bar{J}] = [T_{[0]}] \quad (\text{Def.}) \quad (2.13)$$

where  $[T^{[0]}]$  and  $[T_{[0]}]$  are the Cartesian components of the contra-variant and co-variant stress tensors. Definitions 2.12 and 2.13 with  $|J| = 1$  hold for incompressible matter.  $[T^{[0]}]$  is the second Piola-Kirchhoff stress tensor.

### 2.4 Convected time derivatives of Green's and Almansi strain tensors [1]

Following reference [1] and noting that Green's strain tensor is a co-variant measure whereas Almansi strain tensor is a contra-variant measure, both for finite strain, we can summarize their convected time derivatives in co- and contra-variant bases. These hold for both compressible as well as incompressible matter.

#### Co-variant basis: convected time derivatives of Green's strain tensor $[\varepsilon]$

If  $[\gamma_{(j)}]$ ;  $j = 1, 2, \dots, n$  are the convected time derivatives of  $[\varepsilon]$  of orders  $j = 1, 2, \dots, n$  in co-variant basis and if  $[\gamma_{[j]}]$ ;  $j = 1, 2, \dots, n$  are their Cartesian components in the  $x$ -frame, then following [1] we have

$$\left. \begin{aligned} \frac{D}{Dt}[\gamma_{[k-1]}] &= [\gamma_{[k]}] \\ [\gamma_{[k]}] &= [J]^t[\gamma_{(k)}][J] \\ [\gamma_{(k)}] &= \frac{D}{Dt}[\gamma_{(k-1)}] + [L]^t[\gamma_{(k-1)}] + [\gamma_{(k-1)}][L] \end{aligned} \right\} \quad k = 2, 3, \dots \quad (2.14)$$

and

$$[\gamma_{[1]}] = \frac{D}{Dt}[\varepsilon] = [J]^t[\gamma_{(1)}][J] \quad (2.15)$$

$$[\gamma_{(0)}] = [\gamma_{(1)}] = \frac{1}{2}([L] + [L]^t) \quad (2.16)$$

where  $[\gamma_{(j)}]$ ;  $j = 1, 2, \dots, n$  are fundamental kinematic tensors in the co-variant basis. It is straight forward to show that these are objective.

#### Contra-variant basis: convected time derivatives of Almansi strain tensor $[\bar{\varepsilon}]$

If  $[\gamma^{(j)}]$ ;  $j = 1, 2, \dots, n$  are the convected time derivatives of  $[\bar{\varepsilon}]$  of orders  $j = 1, 2, \dots, n$  in contra-variant basis and if  $[\gamma^{[j]}]$ ;  $j = 1, 2, \dots, n$  are their Cartesian components in the  $x$ -frame, then following [1] we have

$$\left. \begin{aligned} \frac{D}{Dt}[\gamma^{[k-1]}] &= [\gamma^{[k]}] \\ [\gamma^{[k]}] &= [\bar{J}][\gamma^{(k)}][\bar{J}]^t \\ [\gamma^{(k)}] &= \frac{D}{Dt}[\gamma^{(k-1)}] - [L][\gamma^{(k-1)}] - [\gamma^{(k-1)}][L]^t \end{aligned} \right\} \quad k = 2, 3, \dots \quad (2.17)$$

and

$$[\gamma^{[1]}] = \frac{D}{Dt}[\bar{\varepsilon}] = [\bar{J}][\gamma^{(1)}][\bar{J}]^t \quad (2.18)$$

$$[\gamma^{(0)}] = [\gamma^{(1)}] = \frac{1}{2}([L] + [L]^t) \quad (2.19)$$

where  $[\gamma^{(j)}]$ ;  $j = 1, 2, \dots, n$  are fundamental kinematic tensors in the contra-variant basis. These are also objective.

## 2.5 Convected time derivatives of co- and contra-variant Cauchy stress tensors

In this section we summarize the convected time derivatives of co- and contra-variant Cauchy stress tensors for incompressible as well as compressible matter [1].

### Incompressible matter

For incompressible matter  $|J| = 1$  simplifies the convected time derivative expressions.

#### Co-variant basis: Convected time derivatives of co-variant Cauchy stress tensor $[\bar{T}_{(0)}]$

If  $[\bar{T}_{(j)}] ; j = 1, 2, \dots, n$  are the convected time derivatives of orders  $j = 1, 2, \dots, n$  of the co-variant Cauchy stress tensor  $[\bar{T}_{(0)}]$  in the co-variant basis and if  $[T_{[j]}] ; j = 1, 2, \dots, n$  are their Cartesian components in the  $x$ -frame, then following [1] we have

$$\left. \begin{aligned} \frac{D}{Dt}[T_{[k-1]}] &= [T_{[k]}] \\ [T_{[k]}] &= [J]^t [\bar{T}_{(k)}] [J] \\ [\bar{T}_{(k)}] &= \frac{D}{Dt}[\bar{T}_{(k-1)}] + [L]^t [\bar{T}_{(k-1)}] + [\bar{T}_{(k-1)}][L] \end{aligned} \right\} \quad k = 1, 2, \dots \quad (2.20)$$

It can be easily shown that  $[\bar{T}_{(j)}] ; j = 1, 2, \dots, n$  are objective.

#### Contra-variant basis: Convected time derivatives of contra-variant Cauchy stress tensor $[\bar{T}^{(0)}]$

If  $[\bar{T}^{(j)}] ; j = 1, 2, \dots, n$  are the convected time derivatives of orders  $j = 1, 2, \dots, n$  of the contra-variant Cauchy stress tensor  $[\bar{T}^{(0)}]$  in the contra-variant basis and if  $[T^{[j]}] ; j = 1, 2, \dots, n$  are their Cartesian components in the  $x$ -frame, then following [1] we have

$$\left. \begin{aligned} \frac{D}{Dt}[T^{[k-1]}] &= [T^{[k]}] \\ [T^{[k]}] &= [\bar{J}][\bar{T}^{(k)}][\bar{J}]^t \\ [\bar{T}^{(k)}] &= \frac{D}{Dt}[\bar{T}^{(k-1)}] - [L][\bar{T}^{(k-1)}] - [\bar{T}^{(k-1)}][L]^t \end{aligned} \right\} \quad k = 1, 2, \dots \quad (2.21)$$

Tensors  $[\bar{T}^{(j)}] ; j = 1, 2, \dots, n$  are also objective.

### Compressible matter

In case of compressible matter  $|J| \neq 1$ , hence the convected time derivative expression contains additional terms compared to the incompressible case.

#### Co-variant basis: Convected time derivatives of co-variant Cauchy stress tensor $[\bar{T}_{(0)}]$

If  $[\bar{T}_{(j)}] ; j = 1, 2, \dots, n$  are the convected time derivatives of orders  $j = 1, 2, \dots, n$  of the co-variant Cauchy stress tensor  $[\bar{T}_{(0)}]$  in the co-variant basis and if  $[T_{[j]}] ; j = 1, 2, \dots, n$  are their Cartesian components in the  $x$ -frame, then following [1] we have

$$\left. \begin{aligned} \frac{D}{Dt}[T_{[k-1]}] &= [T_{[k]}] \\ [T_{[k]}] &= |J| [J]^t [\bar{T}_{(k)}] [J] \\ [\bar{T}_{(k)}] &= \frac{D}{Dt}[\bar{T}_{(k-1)}] + [L]^t [\bar{T}_{(k-1)}] + [\bar{T}_{(k-1)}][L] + [\bar{T}_{(k-1)}]\text{tr}([L]) \end{aligned} \right\} \quad k = 1, 2, \dots \quad (2.22)$$

It can be easily shown that tensors  $[\bar{T}_{(j)}] ; j = 1, 2, \dots, n$  are objective.

### Contra-variant basis: Convected time derivatives of contra-variant Cauchy stress tensor $[\bar{T}^{(0)}]$

If  $[\bar{T}^{(j)}]$ ;  $j = 1, 2, \dots, n$  are the convected time derivatives of orders  $j = 1, 2, \dots, n$  of the contra-variant Cauchy stress tensor  $[\bar{T}^{(0)}]$  in the contra-variant basis and if  $[T^{[j]}]$ ;  $j = 1, 2, \dots, n$  are their Cartesian components in the  $x$ -frame, then following [1] we have

$$\left. \begin{aligned} \frac{D}{Dt}[T^{[k-1]}] &= [T^{[k]}] \\ [T^{[k]}] &= |J|[\bar{J}][\bar{T}^{(k)}][\bar{J}]^t \\ [\bar{T}^{(k)}] &= \frac{D}{Dt}[\bar{T}^{(k-1)}] - [L][\bar{T}^{(k-1)}] - [\bar{T}^{(k-1)}][L]^t + [\bar{T}^{(k-1)}]\text{tr}([L]) \end{aligned} \right\} \quad k = 1, 2, \dots \quad (2.23)$$

Tensors  $[\bar{T}^{(j)}]$ ;  $j = 1, 2, \dots, n$  are also objective.

## 3 Considerations in the development of the constitutive theory

Amongst many axioms and principles of continuum mechanics [16, 17], the constitutive theory must satisfy conservation laws. Since conservation of mass, balance of momenta and conservation of energy are independent of the constitution of the matter (they assume existence of the stress field and heat vector without regard to how they are arrived at), the second law of thermodynamics, i.e., entropy inequality must be considered in the development of the constitutive theory. Derivation of the entropy inequality in Lagrangian and Eulerian descriptions has been presented in reference [1]. For the sake of brevity, the details are not repeated here. Instead, we borrow the required information from [1]. From the entropy inequality we deduce the following. (i) The conditions that ensure that the entropy inequality is not violated. (ii) We determine the dependent variables in the constitutive theory. (iii) From the conditions resulting from the entropy inequality, we explore the possibility of deriving the constitutive theory. Details are presented in the following.

The choice of Eulerian or Lagrangian form is immaterial for the entropy inequality, hence we choose Lagrangian form [1].

$$\rho \left( \frac{\partial \Phi}{\partial t} + \eta \frac{\partial \theta}{\partial t} \right) + \frac{|J|q_i g_i}{\theta} - \sigma_{ki}^* \dot{J}_{ik} \leq 0 \quad (3.1)$$

We note that in addition to the stress tensor and heat vector that already appear in momentum and energy equations and in 3.1, we have two additional variables  $\Phi$  and  $\eta$ , the Helmholtz free energy density and the entropy density. All other quantities have the usual meaning [1]. Thus we must consider Helmholtz free energy density, entropy density, stress tensor and heat vector as dependent variables in the constitutive theory (in Eulerian as well as Lagrangian descriptions). Since 3.1 contains time derivative of the Helmholtz free energy density, it becomes necessary to determine the arguments of  $\Phi$  and likewise the arguments of the stress tensor  $\sigma$ , entropy density  $\eta$  and heat vector  $q$ .

Based on the principle of equipresence, at the onset we consider all possible measures of deformation as arguments of  $\sigma$ ,  $q$ ,  $\Phi$  and  $\eta$  (or  $\bar{\sigma}$ ,  $\bar{q}$ ,  $\bar{\Phi}$  and  $\bar{\eta}$ ). The Jacobian of deformation  $[J]$  is fundamental in the kinematics and hence must be an argument in each of the four dependent variables. Since we are considering Eulerian description in the rate equations,  $[\dot{J}]$  (time or material derivative of  $[J]$ ) must be in the argument list also. Temperature  $\theta$  is obviously an argument. In addition to these three, we also consider  $g$ , the temperature gradient, as an argument. Thus we have

$$\begin{aligned} \sigma &= \sigma([J], [\dot{J}], \theta, g) \\ q &= q([J], [\dot{J}], \theta, g) \\ \Phi &= \Phi([J], [\dot{J}], \theta, g) \\ \eta &= \eta([J], [\dot{J}], \theta, g) \end{aligned} \quad (3.2)$$

If in 3.2 the independent variables are  $(x_i, t)$ , then these are in Lagrangian or material description in which case  $\sigma$  may represent the first Piola-Kirchhoff stress, or the second Piola-Kirchhoff stress (Cartesian components of the contra-variant Cauchy stress tensor), or the Cartesian components of the co-variant Cauchy stress tensor.

On the other hand, if the independent variables are  $(\bar{x}_i, t)$ , then these are in the Eulerian or spatial description in which case  $\sigma$  may represent contra- or co-variant Cauchy stress tensor.

Now, since we have arguments of  $\Phi$ , we can consider a more detailed form of entropy inequality 3.1 by expanding the time derivative of  $\Phi$ .

$$\frac{\partial \Phi}{\partial t} = \frac{\partial \Phi}{\partial J_{ik}} \dot{J}_{ik} + \frac{\partial \Phi}{\partial \dot{J}_{ik}} \ddot{J}_{ik} + \frac{\partial \Phi}{\partial \theta} \dot{\theta} + \frac{\partial \Phi}{\partial g_i} \dot{g}_i \quad (3.3)$$

Substituting 3.3 in 3.1

$$\rho \left( \frac{\partial \Phi}{\partial J_{ik}} \dot{J}_{ik} + \frac{\partial \Phi}{\partial \dot{J}_{ik}} \ddot{J}_{ik} + \frac{\partial \Phi}{\partial \theta} \dot{\theta} + \frac{\partial \Phi}{\partial g_i} \dot{g}_i + \eta \frac{\partial \theta}{\partial t} \right) + \frac{|J| \underline{q}_i \underline{g}_i}{\theta} - \sigma_{ki}^* \dot{J}_{ik} \leq 0 \quad (3.4)$$

$$\text{or } \rho \frac{\partial \Phi}{\partial \dot{J}_{ik}} \ddot{J}_{ik} + \left( \rho \frac{\partial \Phi}{\partial J_{ik}} - \sigma_{ki}^* \right) \dot{J}_{ik} + \rho \left( \frac{\partial \Phi}{\partial \theta} + \eta \right) \dot{\theta} + \frac{|J| \underline{q}_i \underline{g}_i}{\theta} + \frac{\partial \Phi}{\partial g_i} \dot{g}_i \leq 0 \quad (3.5)$$

In order for 3.5 to hold for arbitrary (but admissible)  $[\ddot{J}]$ ,  $\dot{\theta}$  and  $\dot{\mathbf{g}}$  the following must hold:

$$\rho \frac{\partial \Phi}{\partial \dot{J}_{ik}} = 0 \quad (3.6)$$

$$\frac{\partial \Phi}{\partial g_i} = 0 \quad (3.7)$$

$$\frac{\partial \Phi}{\partial \theta} + \eta = 0 \quad (3.8)$$

$$\text{and } \left( \rho \frac{\partial \Phi}{\partial J_{ik}} - \sigma_{ki}^* \right) \dot{J}_{ik} + \frac{|J| \underline{q}_i \underline{g}_i}{\theta} \leq 0 \quad (3.9)$$

Equations 3.6 - 3.9 are fundamental relations from the second law of thermodynamics (or entropy inequality).

**Remarks:**

- (1) 3.6 implies that  $\Phi$  is not a function of  $[\dot{J}]$ .
- (2) 3.7 implies that  $\Phi$  is not a function of  $\mathbf{g}$  either.
- (3) Based on 3.8,  $\eta$  is not a dependent variable in the constitutive theory as  $\eta = -\frac{\partial \Phi}{\partial \theta}$ , hence  $\eta$  is deterministic from  $\Phi$ .
- (4) The inequality in the last equation 3.9 is essential in the form it is stated. For example,

$$\rho \frac{\partial \Phi}{\partial J_{ik}} - \sigma_{ki}^* = 0 \quad \text{and} \quad \frac{|J| \underline{q}_i \underline{g}_i}{\theta} \leq 0$$

are inappropriate due to the fact that these imply that  $[\sigma^*]$  is not a function of  $[\dot{J}]$  which is contrary to 3.2. Thus 3.9 in its stated form is unable to provide us further details regarding the constitutive theory for  $[\sigma^*]$  and  $\mathbf{q}$ .

In order to alleviate the situation discussed in remark (4), we consider decomposition of  $[\sigma^*]$  into equilibrium stress  $[_e\sigma^*]$  and deviatoric stress  $[_d\sigma^*]$ , i.e.

$$[\sigma^*] = [_e\sigma^*] + [_d\sigma^*] \quad (3.10)$$

At this stage we can only conclude the following:

$$[_e\sigma^*] = [_e\sigma^*]([J], [0], \theta, \mathbf{g}) \quad (3.11)$$

$$[_d\sigma^*] = [_d\sigma^*]([J], [\dot{J}], \theta, \mathbf{g}) \quad (3.12)$$

That is,  $[_e\sigma^*]$  is not a function of  $[\dot{J}]$  and  $[_d\sigma^*]$  vanishes when  $[\dot{J}]$  and  $\mathbf{g}$  are zero. Substituting 3.10 into 3.9 gives

$$\left( \rho \frac{\partial \Phi}{\partial J_{ik}} - {}_e\sigma_{ki}^* - {}_d\sigma_{ki}^* \right) \dot{J}_{ik} + \frac{|J| \underline{q}_i \underline{g}_i}{\theta} \leq 0 \quad (3.13)$$

Since  $\Phi$  is not a function of  $[\dot{J}]$  and neither is  ${}_e\sigma_{ik}^*$  (3.11), then  ${}_e\sigma_{ik}^*$  must be derivable from

$${}_e\sigma_{ki}^* = \rho \frac{\partial \Phi}{\partial J_{ik}} \quad (3.14)$$

Using 3.14, the inequality 3.13 reduces to

$$-{}_d\sigma_{ki}^* \dot{J}_{ik} + \frac{|J| \underline{q}_i \underline{g}_i}{\theta} \leq 0 \quad (3.15)$$

If we assume (as done routinely to derive Fourier heat conduction law [1, 16–18])

$$\frac{|J| \underline{q}_i \underline{g}_i}{\theta} \leq 0 \quad (3.16)$$

Then 3.15 is satisfied if the following holds.

$${}_d\sigma_{ki}^* \dot{J}_{ik} > 0 \quad (3.17)$$

Equation 3.17 requires that conversion of mechanical energy must be positive. Thus 3.10 can be written as

$$\sigma_{ij}^* = \rho \frac{\partial \Phi}{\partial J_{ki}} + {}_d\sigma_{ij}^*([J], [\dot{J}], \theta, \mathbf{g}) \quad (3.18)$$

$$\text{and} \quad \Phi = \Phi([J], \theta) \quad (3.19)$$

$$\mathbf{q} = \mathbf{q}([J], [\dot{J}], \theta, \mathbf{g}) \quad (3.20)$$

Derivation of Fourier heat conduction law for  $\mathbf{q}$  is straight forward based on 3.16 [1, 16–18]. A more general derivation based on 3.20 is presented in a subsequent section.

### Further consideration on argument tensors

We note that in Eulerian description, transformation of its reference frame by a unimodular (orthogonal) matrix cannot be detected by its subsequent thermomechanical deformation. Thus if  $x$ -frame changes to  $x'$ -frame via

$$\{x'\} = [R]\{x\} \quad (3.21)$$

$$\therefore [J'] = [J][R]^t \quad (3.22)$$

Then, based on the principle of frame invariance

$$\Phi([J], \theta) = \Phi([J'], \theta) = \Phi([J][R]^t, \theta) \quad (3.23)$$

must hold and likewise, the principle of frame invariance must also hold for the stress tensor and heat vector. But this is only possible if  $\Phi$ , the stress tensor and heat vector depend upon  $|J|$  and not  $[J]$  due to the fact that

$$\det[J'] = \det([J][R]^t) = \det[J] \det[R]^t = \det[J] \quad (3.24)$$

is frame invariant. Furthermore, we note that

$$\begin{aligned} [\dot{J}] &= [L][J] \quad ; \quad [D] = \frac{1}{2}([L] + [L]^t) \quad ; \quad [W] = \frac{1}{2}([L] - [L]^t) \\ \therefore [L] &= [D] + [W] \quad \text{and} \quad [\dot{J}] = ([D] + [W])[J] \end{aligned} \quad (3.25)$$

Thus, dependence of the stress tensor and heat vector on  $[\dot{J}]$  can be replaced by the dependence on  $|J|$ ,  $[D]$  and  $[W]$ . But  $[W]$  is pure rotation and hence dependence on  $[W]$  can be eliminated. Thus, the stress tensor and heat vector must have dependence on  $|J|$ ,  $[D]$ ,  $\theta$  and  $\mathbf{g}$ . We observe the following:

- (1) From conservation of mass

$$\rho = |J|\bar{\rho} \quad \text{or} \quad |J| = \frac{\rho}{\bar{\rho}} \quad (3.26)$$

in which  $\rho$  is constant (density in the reference configuration). Thus  $|J|$  can be replaced with  $1/\bar{\rho}$  or simply  $\bar{\rho}$ .

- (2) Since for fluids, Eulerian description is necessary, we have two obvious choices: contra-variant basis or co-variant basis and hence contra-variant Cauchy stress  $[\bar{\sigma}^{(0)}]$  or co-variant Cauchy stress  $[\bar{\sigma}_{(0)}]$  tensors are obvious choices in the constitutive theory.
- (3) Recalling the derivations of the convected time derivatives of Green's strain in the co-variant basis, we note that  $[D]$  is the convected time derivative of order one of the Green's strain in the co-variant basis, i.e.

$$[D] = [\gamma_{(1)}] \quad (3.27)$$

which is also the convected time derivative of order zero (by definition). Thus

$$[D] = [\gamma_{(0)}] = [\gamma_{(1)}] \quad (3.28)$$

By definition,  $[\gamma_{(0)}]$  and  $[\gamma_{(1)}]$  are fundamental kinematic tensors of order zero and one in co-variant basis based on Green's strain tensor, a co-variant measure of finite strain.

- (4) Likewise if we consider the convected time derivatives of the Almansi strain in contra-variant basis, we note that  $[D]$  is also the convected time derivative of order one of the Almansi strain in contra-variant basis, i.e.

$$[D] = [\gamma^{(1)}] \quad (3.29)$$

which is also the convected time derivative of order zero (by definition). Thus

$$[D] = [\gamma^{(0)}] = [\gamma^{(1)}] \quad (3.30)$$

By definition,  $[\gamma^{(0)}]$  and  $[\gamma^{(1)}]$  are fundamental kinematic tensors of order zero and one in contra-variant basis derived using Almansi strain tensor, a contra-variant measure of finite strain.

- (5) We have seen that convected time derivatives of order higher than one of the Green's strain tensor and Almansi strain tensor can be derived in co-variant and contra-variant bases which are fundamental kinematic tensors of various orders in the respective bases. Thus

$$[\gamma^{(j)}] \quad ; \quad j = 1, 2, \dots, n \quad (3.31)$$

$$\text{and} \quad [\gamma_{(j)}] \quad ; \quad j = 1, 2, \dots, n \quad (3.32)$$

are fundamental kinematic tensors in contra- and co-variant bases which must be considered in the constitutive theory and hence these must replace  $[D]$  in the argument tensors for the dependent variables in the constitutive theory.

With considerations (1) to (5), we now have finalized the dependent variables and their argument tensors in the constitutive theory.

In Eulerian description, co-variant and contra-variant bases are obviously two clear choices for the development of the constitutive theory. In the following we consider these two bases and the choice of dependent variables in the constitutive theory and their argument tensors for compressible and incompressible cases.

### 3.1 Final choice of the argument tensors: compressible

#### Contra-variant basis:

The conjugate pairs of the Cauchy stress tensor and fundamental kinematic tensor in the contra-variant basis are

$$[\bar{\sigma}^{(0)}] \quad , \quad [\gamma^{(j)}] \quad ; \quad j = 1, 2, \dots, n \quad (3.33)$$

and we have the following for the dependent variables in the constitutive theory.

$$\bar{\Phi} = \bar{\Phi}(\bar{\rho}(\bar{\mathbf{x}}, t), \bar{\theta}(\bar{\mathbf{x}}, t)) \quad (3.34)$$

$$[\bar{\sigma}^{(0)}] = [\bar{\sigma}^{(0)}(\bar{\rho}(\bar{\mathbf{x}}, t), [\gamma^{(j)}(\bar{\mathbf{x}}, t)]; j = 1, 2, \dots, n, \bar{\theta}(\bar{\mathbf{x}}, t), \bar{\mathbf{g}}(\bar{\mathbf{x}}, t))] \quad (3.35)$$

$$[\bar{\sigma}^{(0)}] = [{}_e\bar{\sigma}^{(0)}] + [{}_d\bar{\sigma}^{(0)}(\bar{\rho}(\bar{\mathbf{x}}, t), [\gamma^{(j)}(\bar{\mathbf{x}}, t)]; j = 1, 2, \dots, n, \bar{\theta}(\bar{\mathbf{x}}, t), \bar{\mathbf{g}}(\bar{\mathbf{x}}, t))] \quad (3.36)$$

$$\bar{\mathbf{q}}^{(0)} = \bar{\mathbf{q}}^{(0)}(\bar{\rho}(\bar{\mathbf{x}}, t), [\gamma^{(j)}(\bar{\mathbf{x}}, t)]; j = 1, 2, \dots, n, \bar{\theta}(\bar{\mathbf{x}}, t), \bar{\mathbf{g}}(\bar{\mathbf{x}}, t)) \quad (3.37)$$

$$[{}_e\sigma^*]^t = \rho(\mathbf{x}, t) \frac{\partial \Phi(\rho(\mathbf{x}, t), \theta(\mathbf{x}, t))}{\partial [J(\mathbf{x}, t)]} \quad (3.38)$$

In 3.36, the contra-variant Cauchy stress tensor  $[\bar{\sigma}^{(0)}]$  has been decomposed into the equilibrium stress tensor  $[{}_e\bar{\sigma}^{(0)}]$  and the deviatoric Cauchy stress tensor  $[{}_d\bar{\sigma}^{(0)}]$ .

### Co-variant basis:

The conjugate pairs of Cauchy stress tensor and fundamental kinematic tensors in the co-variant basis are

$$[\bar{\sigma}_{(0)}] \quad , \quad [\gamma_{(j)}] \quad ; \quad j = 1, 2, \dots, n \quad (3.39)$$

and we have the following for the dependent variables in the constitutive theory.

$$\bar{\Phi} = \bar{\Phi}(\bar{\rho}(\bar{\mathbf{x}}, t), \bar{\theta}(\bar{\mathbf{x}}, t)) \quad (3.40)$$

$$[\bar{\sigma}_{(0)}] = [\bar{\sigma}_{(0)}(\bar{\rho}(\bar{\mathbf{x}}, t), [\gamma_{(j)}(\bar{\mathbf{x}}, t)]; j = 1, 2, \dots, n, \bar{\theta}(\bar{\mathbf{x}}, t), \bar{\mathbf{g}}(\bar{\mathbf{x}}, t))] \quad (3.41)$$

$$[\bar{\sigma}_{(0)}] = [{}_e\bar{\sigma}_{(0)}] + [{}_d\bar{\sigma}_{(0)}(\bar{\rho}(\bar{\mathbf{x}}, t), [\gamma_{(j)}(\bar{\mathbf{x}}, t)]; j = 1, 2, \dots, n, \bar{\theta}(\bar{\mathbf{x}}, t), \bar{\mathbf{g}}(\bar{\mathbf{x}}, t))] \quad (3.42)$$

$$\bar{\mathbf{q}}_{(0)} = \bar{\mathbf{q}}_{(0)}(\bar{\rho}(\bar{\mathbf{x}}, t), [\gamma_{(j)}(\bar{\mathbf{x}}, t)]; j = 1, 2, \dots, n, \bar{\theta}(\bar{\mathbf{x}}, t), \bar{\mathbf{g}}(\bar{\mathbf{x}}, t)) \quad (3.43)$$

$$[{}_e\sigma^*]^t = \rho(\mathbf{x}, t) \frac{\partial \Phi(\rho(\mathbf{x}, t), \theta(\mathbf{x}, t))}{\partial [J(\mathbf{x}, t)]} \quad (3.44)$$

In 3.42, the co-variant Cauchy stress tensor  $[\bar{\sigma}_{(0)}]$  has been decomposed into the equilibrium stress tensor  $[{}_e\bar{\sigma}_{(0)}]$  and the deviatoric Cauchy stress tensor  $[{}_d\bar{\sigma}_{(0)}]$ .

## 3.2 Final choice of the argument tensors: incompressible

For incompressible matter  $\bar{\rho} = \rho = \text{constant}$ . Thus we have the following for contra-variant and co-variant bases.

### Contra-variant basis:

The conjugate pairs of the Cauchy stress tensor and fundamental kinematic tensor in the contra-variant basis are

$$[\bar{\sigma}^{(0)}] \quad , \quad [\gamma^{(j)}] \quad ; \quad j = 1, 2, \dots, n \quad (3.45)$$

The derivation of  $[{}_e\sigma^*]$  for incompressible matter presented in reference [1] holds here precisely and hence is omitted. Thus we have the following for the dependent variables in the constitutive theory.

$$\bar{\Phi} = \bar{\Phi}(\bar{\theta}(\bar{\mathbf{x}}, t)) \quad (3.46)$$

$$[\bar{\sigma}^{(0)}] = [\bar{\sigma}^{(0)}([\gamma^{(j)}(\bar{\mathbf{x}}, t)]; j = 1, 2, \dots, n, \bar{\theta}(\bar{\mathbf{x}}, t), \bar{\mathbf{g}}(\bar{\mathbf{x}}, t))] \quad (3.47)$$

$$[\bar{\sigma}^{(0)}] = [{}_e\bar{\sigma}^{(0)}] + [{}_d\bar{\sigma}^{(0)}([\gamma^{(j)}(\bar{\mathbf{x}}, t)]; j = 1, 2, \dots, n, \bar{\theta}(\bar{\mathbf{x}}, t), \bar{\mathbf{g}}(\bar{\mathbf{x}}, t))] \quad (3.48)$$

$$\bar{\mathbf{q}}^{(0)} = \bar{\mathbf{q}}^{(0)}([\gamma^{(j)}(\bar{\mathbf{x}}, t)]; j = 1, 2, \dots, n, \bar{\theta}(\bar{\mathbf{x}}, t), \bar{\mathbf{g}}(\bar{\mathbf{x}}, t)) \quad (3.49)$$

$$[{}_e\sigma^*] = p(\theta(\mathbf{x}, t))[J(\mathbf{x}, t)]^{-1} \quad (3.50)$$

### Co-variant basis:

The conjugate pairs of stress tensor and fundamental kinematic tensors in the co-variant basis are

$$[\bar{\sigma}_{(0)}] \quad , \quad [\gamma_{(j)}] \quad ; \quad j = 1, 2, \dots, n \quad (3.51)$$

As in the case of contra-variant basis, the derivation of  $[_e\sigma^*]$  for incompressible matter presented in reference [1] holds here precisely. Thus we have the following for the dependent variables in the constitutive theory.

$$\bar{\Phi} = \bar{\Phi}(\bar{\theta}(\bar{\mathbf{x}}, t)) \quad (3.52)$$

$$[\bar{\sigma}_{(0)}] = [\bar{\sigma}_{(0)}(\gamma_{(j)}(\bar{\mathbf{x}}, t); j = 1, 2, \dots, n, \bar{\theta}(\bar{\mathbf{x}}, t), \bar{\mathbf{g}}(\bar{\mathbf{x}}, t))] \quad (3.53)$$

$$[\bar{\sigma}_{(0)}] = [_e\bar{\sigma}_{(0)}] + [_d\bar{\sigma}_{(0)}(\gamma_{(j)}(\bar{\mathbf{x}}, t); j = 1, 2, \dots, n, \bar{\theta}(\bar{\mathbf{x}}, t), \bar{\mathbf{g}}(\bar{\mathbf{x}}, t))] \quad (3.54)$$

$$\bar{\mathbf{q}}_{(0)} = \bar{\mathbf{q}}_{(0)}(\gamma_{(j)}(\bar{\mathbf{x}}, t); j = 1, 2, \dots, n, \bar{\theta}(\bar{\mathbf{x}}, t), \bar{\mathbf{g}}(\bar{\mathbf{x}}, t)) \quad (3.55)$$

$$[_e\sigma^*] = p(\theta(\mathbf{x}, t))[J(\mathbf{x}, t)]^{-1} \quad (3.56)$$

In the following sections we consider specific details of the rate constitutive theory in the two bases for compressible and incompressible cases.

## 4 Development of the rate constitutive theory for the stress tensor

### 4.1 Equilibrium stress $[_e\bar{\sigma}^{(0)}]$ or $[_e\bar{\sigma}_{(0)}]$

The development of the constitutive equations for the equilibrium stress requires the use of 3.14 and transformation of  $[_e\sigma^*]$  to  $[_e\bar{\sigma}^{(0)}]$  or  $[_e\bar{\sigma}_{(0)}]$ . The derivation presented in reference [1] holds here precisely and hence is not repeated. We only present the final forms.

#### Compressible solid matter:

$$[_e\bar{\sigma}^{(0)}] = [_e\bar{\sigma}_{(0)}] = p(\bar{\rho}, \bar{\theta})[I] \quad (4.1)$$

i.e., equilibrium stress is independent of the choice of basis.  $p(\bar{\rho}, \bar{\theta})$  is thermodynamic pressure defined by the equation of state.

#### Incompressible solid matter:

$$[_e\bar{\sigma}^{(0)}] = [_e\bar{\sigma}_{(0)}] = p(\bar{\theta})[I] \quad (4.2)$$

$p(\bar{\theta})$  is mechanical pressure.  $p(\bar{\theta})$  is not deterministic from the deformation field.

In 4.1 and 4.2 we can replace  $p(\bar{\rho}, \bar{\theta})$  and  $p(\bar{\theta})$  by  $-p(\bar{\rho}, \bar{\theta})$  and  $-p(\bar{\theta})$  if we define the compressive pressure to be positive.

### 4.2 Deviatoric Cauchy stress $[_d\bar{\sigma}^{(0)}]$ or $[_d\bar{\sigma}_{(0)}]$

In this section we consider the constitutive theory for the deviatoric Cauchy stress in contra- and co-variant bases.

#### Compressible solid matter:

Based on 3.36, 4.1 and 3.42, 4.1 we have the following for compressible thermoelastic solids:

$$[\bar{\sigma}^{(0)}] = p(\bar{\rho}, \bar{\theta})[I] + [_d\bar{\sigma}^{(0)}(\bar{\rho}, [\gamma_{(j)}]; j = 1, 2, \dots, n, \bar{\theta}, \bar{\mathbf{g}})] \quad (4.3)$$

$$[\bar{\sigma}_{(0)}] = p(\bar{\rho}, \bar{\theta})[I] + [_d\bar{\sigma}_{(0)}(\bar{\rho}, [\gamma_{(j)}]; j = 1, 2, \dots, n, \bar{\theta}, \bar{\mathbf{g}})] \quad (4.4)$$

### Incompressible solid matter:

Based on 3.48, 4.2 and 3.54, 4.2 we have the following for incompressible thermoelastic solids:

$$[\bar{\sigma}^{(0)}] = p(\bar{\theta})[I] + [{}_d\bar{\sigma}^{(0)}([\gamma^{(j)}]; j = 1, 2, \dots, n, \bar{\theta}, \bar{\mathbf{g}})] \quad (4.5)$$

$$[\bar{\sigma}_{(0)}] = p(\bar{\theta})[I] + [{}_d\bar{\sigma}_{(0)}([\gamma_{(j)}]; j = 1, 2, \dots, n, \bar{\theta}, \bar{\mathbf{g}})] \quad (4.6)$$

First, we make some remarks [1] that are helpful in understanding the approach used for deriving the constitutive equations for the deviatoric stress:

- (1)  $[\gamma_{(j)}]$  and  $[\gamma^{(j)}]; j = 1, 2, \dots, n$  are fundamental kinematic tensors of rank two;  $\bar{\rho}, \bar{\theta}$  are tensors of rank zero and  $\bar{\mathbf{g}}$  is a tensor of rank one.
- (2)  $[\gamma_{(j)}], [\gamma^{(j)}]; j = 1, 2, \dots, n$  and  $\bar{\mathbf{g}}$  have their own invariants but also there exist combined invariants between them.
- (3) In the case of homogeneous and isotropic elastic compressible matter, the equilibrium stress is completely deterministic from the entropy inequality once we define Helmholtz free energy density in terms of the invariants of the chosen strain measure. This yields thermodynamic pressure  $p(\bar{\rho}, \bar{\theta})$ . In the case of isotropic elastic incompressible matter, the equilibrium stress is also derived from the entropy inequality, however, it is not a function of the Helmholtz free energy density and thus it is not deterministic from the deformation field. Furthermore, the second law of thermodynamics only restricts the dissipative energy (entropy production) due to the deviatoric Cauchy stress to be positive but provides no mechanism for determining the constitutive theory for the deviatoric Cauchy stress.
- (4) The theory of generators and invariants [19–29] provides a continuum mechanics foundation to derive constitutive theory for the deviatoric Cauchy stress. This theory utilizes a linear combination of the combined generators (that are symmetric and are of the same rank as the deviatoric Cauchy stress) of the argument tensors of rank one and two to describe the deviatoric Cauchy stress tensor field. The coefficients in the linear combinations are functions of combined invariants of the argument tensors, temperature  $\bar{\theta}$  and density  $\bar{\rho}$  which are then determined by using Taylor series expansion of the coefficients about the reference configuration. Thus, in principle, this approach is quite straight forward.
- (5) Based on (4), the key element in the theory of generators and invariants is the determination of the minimal basis based on the combined generators of the argument tensors and of course, determination of the combined invariants. For example  $[T([S])] where  $[T]$  and  $[S]$  are symmetric tensors of rank two which obey invariance$

$$[T([R][S][R]^t)] = [R][T([S])][R]^t \quad (4.7)$$

has the form

$$[T] = \alpha_0[I] + \alpha_1[S] + \alpha_2[S]^2 \quad (4.8)$$

where  $\alpha_0, \alpha_1$  and  $\alpha_2$  are functions of the invariants of  $[S]$ , i.e.,  $\text{tr}([S]), \text{tr}([S]^2)$  and  $\text{tr}([S]^3)$  called principal invariants, or the invariants  $I_s, \mathbb{I}_s$  and  $\mathbb{III}_s$  from the characteristic equation of  $[S]$ . The tensors  $[I], [S], [S]^2$  are called generators of the tensor  $[T]$  and form the minimal basis. If the arguments of  $[T]$  consist of more than one tensor (could be of different rank), then a linear combination like 4.8 would contain all combined generators (of the same rank as  $[T]$ ) of the argument tensors and likewise the coefficients in the linear combination would be functions of the combined invariants. For details on the combined generators and invariants for various combinations of the argument tensors see references [19–29].

- (6) Based on the remarks presented above, we now have a mechanism for deriving constitutive theory for the deviatoric stress as well as the heat vector. In the following we consider contra-variant as well as co-variant bases, keeping in mind that the heat vector is a tensor of rank one and hence the combined generators of its argument tensors must also be of the same rank.
- (7) Before we proceed further we note that when we consider thermoelastic solids in Lagrangian description, the constitutive equations for the stress field (co- or contra-variant basis) are relations that express

dependence of the stress field on the chosen strain measures. However, in Eulerian description, the strain measures are not available. Instead we have first and higher order convected time derivatives of the chosen strain measures. Thus the constitutive equations must describe a relationship between convected time derivatives of the chosen strain measures and the convected time derivative of the corresponding conjugate stress measure. For compressible solid matter, we consider the first convected time derivative of the deviatoric Cauchy stress tensor in contra- and co-variant basis as a dependent variable in the constitutive theory. Its argument tensors are given by

$$[{}_d\bar{\sigma}^{(1)}] = [{}_d\bar{\sigma}^{(1)}(\bar{\rho}, [\gamma^{(j)}]; j = 1, 2, \dots, n, \bar{\theta}, \bar{\mathbf{g}})] \quad (4.9)$$

$$[{}_d\bar{\sigma}_{(1)}] = [{}_d\bar{\sigma}_{(1)}(\bar{\rho}, [\gamma_{(j)}]; j = 1, 2, \dots, n, \bar{\theta}, \bar{\mathbf{g}})] \quad (4.10)$$

For the incompressible case, density is constant, hence 4.9 and 4.10 reduce to 4.11 and 4.12 in contra- and co-variant bases.

$$[{}_d\bar{\sigma}^{(1)}] = [{}_d\bar{\sigma}^{(1)}([\gamma^{(j)}]; j = 1, 2, \dots, n, \bar{\theta}, \bar{\mathbf{g}})] \quad (4.11)$$

$$[{}_d\bar{\sigma}_{(1)}] = [{}_d\bar{\sigma}_{(1)}([\gamma_{(j)}]; j = 1, 2, \dots, n, \bar{\theta}, \bar{\mathbf{g}})] \quad (4.12)$$

4.9 - 4.12 must form the basis for deriving the constitutive theory for the deviatoric Cauchy stress in contra- and co-variant bases. In the following we present details of the constitutive equations based on 4.9 - 4.12 for compressible and incompressible thermoelastic solid matter in contra- and co-variant bases using theory of generators and invariants.

## 5 Development of the constitutive equations for the deviatoric Cauchy stress tensor: compressible

### 5.1 Thermoelastic solids of order two: compressible

#### Contra-variant basis:

In the general theory, we express  $[{}_d\bar{\sigma}^{(1)}]$ , the first convected time derivative of the contra-variant deviatoric Cauchy stress as a linear combinations of the combined generators of the argument tensors  $[\gamma^{(j)}]; j = 1, 2, \dots, n$  and  $\bar{\mathbf{g}}$ . The tensor  $[{}_d\bar{\sigma}^{(1)}]$  for compressible matter can be obtained by replacing  $[\bar{T}^{(1)}]$  with  $[{}_d\bar{\sigma}^{(1)}]$  in 2.23. Since  $[{}_d\bar{\sigma}^{(1)}]$  is a symmetric tensor of rank two, the combined generators  $[16, 17, 19-29]$  of  $[\gamma^{(j)}]; j = 1, 2, \dots, n$  (symmetric tensors of rank two) and  $\bar{\mathbf{g}}$  (tensor of rank one) must be symmetric tensors of rank two. In the derivation presented in the following we limit the argument tensors  $[\gamma^{(j)}]; j = 1, 2, \dots, n$  to just the first two, i.e., we only consider  $[\gamma^{(1)}]$  and  $[\gamma^{(2)}]$ . Table 3.1 lists the combined generators. The combined invariants  $[16, 17, 19-29]$  are listed in table 3.2. Generalization to more than two strain rate tensors presents no difficulty but becomes cumbersome due to the increased number of generators. Hence, for this choice we have

$$[{}_d\bar{\sigma}^{(1)}] = [{}_d\bar{\sigma}^{(1)}(\bar{\rho}, [\gamma^{(1)}], [\gamma^{(2)}], \bar{\theta}, \bar{\mathbf{g}})] \quad (5.1)$$

#### Remarks:

- (i) We note that the invariants listed in table 3.2 under (2) ( marked (a) ) need not be included due to the fact that

$$\text{tr}([\gamma^{(1)}][\gamma^{(2)}] + [\gamma^{(2)}][\gamma^{(1)}]) + \text{tr}([\gamma^{(1)}][\gamma^{(2)}] - [\gamma^{(2)}][\gamma^{(1)}]) = 2\text{tr}([\gamma^{(1)}][\gamma^{(2)}])$$

which is same as  ${}^{q\sigma}\tilde{I}^8$  (except for the factor 2, which is of no consequence). In many published works (a) are also included in addition to  ${}^{q\sigma}\tilde{I}^8$  which is redundant [18] and is in conflict with the minimal basis.

- (ii) Likewise, in many published works  ${}^{q\sigma}\tilde{I}^{16}$  is replaced with two invariants listed under item (3) ( marked (b) ). Following (i), the sum of the invariants marked (b) is two times  ${}^{q\sigma}\tilde{I}^{16}$ . Hence including these in place of  ${}^{q\sigma}\tilde{I}^{16}$  is inappropriate as well (in conflict with minimal basis).

Table 3.1: Combined generators for  $[_d\bar{\sigma}^{(1)}]$ 

Arguments	Generators
(1) none	$[I]$
(2) one at a time ( including (1) )	
$[\gamma^{(1)}]$	$[\sigma\tilde{G}^1] = [\gamma^{(1)}] \quad ; \quad [\sigma\tilde{G}^2] = [\gamma^{(1)}]^2$
$[\gamma^{(2)}]$	$[\sigma\tilde{G}^3] = [\gamma^{(2)}] \quad ; \quad [\sigma\tilde{G}^4] = [\gamma^{(2)}]^2$
$\bar{\mathbf{g}}$	$[\sigma\tilde{G}^5] = \bar{\mathbf{g}} \otimes \bar{\mathbf{g}}$
(3) two at a time ( including (1) and (2) )	
$[\gamma^{(1)}] \quad , \quad [\gamma^{(2)}]$	$[\sigma\tilde{G}^6] = [\gamma^{(1)}][\gamma^{(2)}] + [\gamma^{(2)}][\gamma^{(1)}]$ $[\sigma\tilde{G}^7] = [\gamma^{(1)}]^2[\gamma^{(2)}] + [\gamma^{(2)}][\gamma^{(1)}]^2$ $[\sigma\tilde{G}^8] = [\gamma^{(1)}][\gamma^{(2)}]^2 + [\gamma^{(2)}]^2[\gamma^{(1)}]$
$[\gamma^{(1)}] \quad , \quad \bar{\mathbf{g}}$	$[\sigma\tilde{G}^9] = \bar{\mathbf{g}} \otimes [\gamma^{(1)}]\bar{\mathbf{g}} + [\gamma^{(1)}]\bar{\mathbf{g}} \otimes \bar{\mathbf{g}}$ $[\sigma\tilde{G}^{10}] = \bar{\mathbf{g}} \otimes [\gamma^{(1)}]^2\bar{\mathbf{g}} + [\gamma^{(1)}]^2\bar{\mathbf{g}} \otimes \bar{\mathbf{g}}$
$[\gamma^{(2)}] \quad , \quad \bar{\mathbf{g}}$	$[\sigma\tilde{G}^{11}] = \bar{\mathbf{g}} \otimes [\gamma^{(2)}]\bar{\mathbf{g}} + [\gamma^{(2)}]\bar{\mathbf{g}} \otimes \bar{\mathbf{g}}$ $[\sigma\tilde{G}^{12}] = \bar{\mathbf{g}} \otimes [\gamma^{(2)}]^2\bar{\mathbf{g}} + [\gamma^{(2)}]^2\bar{\mathbf{g}} \otimes \bar{\mathbf{g}}$

Now we can express  $[_d\bar{\sigma}^{(1)}]$  as a linear combination of  $[I]$  and the combined generators  $[\sigma\tilde{G}^i] ; i = 1, 2, \dots, 12$ .

$$[_d\bar{\sigma}^{(1)}] = \sigma_{\alpha^0}[I] + \sum_{i=1}^{12} \sigma_{\alpha^i}[\sigma\tilde{G}^i] \quad (5.2)$$

The coefficients  $\sigma_{\alpha^i} ; i = 0, 1, \dots, 12$  are functions of the combined invariants  ${}^{q\sigma}\tilde{I}^j ; j = 1, 2, \dots, 16$ , density  $\bar{\rho}$  and temperature  $\bar{\theta}$ . The coefficients  $\sigma_{\alpha^i} ; i = 0, 1, \dots, 12$  are determined by using Taylor series expansion for each  $\sigma_{\alpha^i}$  about the reference configuration and only retaining up to linear terms in the combined invariants and  $\bar{\theta}$ .

$$\sigma_{\alpha^i} = \sigma_{\alpha^i} \Big|_{\text{ref}} + \sum_{j=1}^{16} \frac{\partial(\sigma_{\alpha^i})}{\partial({}^{q\sigma}\tilde{I}^j)} \Big|_{\text{ref}} ({}^{q\sigma}\tilde{I}^j - ({}^{q\sigma}\tilde{I}^j)_0) + \frac{\partial(\sigma_{\alpha^i})}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 0, 1, \dots, 12 \quad (5.3)$$

in which the quantities with the subscript zero are their values in the reference configuration. We note that  $({}^{q\sigma}\tilde{I}^j)_0 ; j = 1, 2, \dots, 16$  are all zero due to the fact that  $[\gamma^{(1)}]$  and  $[\gamma^{(2)}]$  are null in the reference configuration (solid at rest, i.e., no motion) and  $\bar{\mathbf{g}}|_0 = 0$  if the solid only has uniform temperature field. Hence 5.3 can be written as

$$\sigma_{\alpha^i} = \sigma_{\alpha^i} \Big|_{\text{ref}} + \sum_{j=1}^{16} \frac{\partial(\sigma_{\alpha^i})}{\partial({}^{q\sigma}\tilde{I}^j)} \Big|_{\text{ref}} {}^{q\sigma}\tilde{I}^j + \frac{\partial(\sigma_{\alpha^i})}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 0, 1, \dots, 12 \quad (5.4)$$

Table 3.2: Combined invariants for  $[_{d\bar{\sigma}}^{(1)}]$ : These are also valid for the heat vector  $\bar{\mathbf{q}}^{(0)}$

Arguments	Invariants
(1) one at a time	
$[\gamma^{(1)}]$	$q\sigma \tilde{I}^1 = \text{tr}([\gamma^{(1)}])$ ; $q\sigma \tilde{I}^2 = \text{tr}([\gamma^{(1)}]^2)$ $q\sigma \tilde{I}^3 = \text{tr}([\gamma^{(1)}]^3)$
$[\gamma^{(2)}]$	$q\sigma \tilde{I}^4 = \text{tr}([\gamma^{(2)}])$ ; $q\sigma \tilde{I}^5 = \text{tr}([\gamma^{(2)}]^2)$ $q\sigma \tilde{I}^6 = \text{tr}([\gamma^{(2)}]^3)$
$\bar{\mathbf{g}}$	$q\sigma \tilde{I}^7 = \bar{\mathbf{g}} \cdot \bar{\mathbf{g}}$
(2) two at a time ( including (1) )	
$[\gamma^{(1)}]$ , $[\gamma^{(2)}]$	$q\sigma \tilde{I}^8 = \text{tr}([\gamma^{(1)}][\gamma^{(2)}])$ ; $q\sigma \tilde{I}^9 = \text{tr}([\gamma^{(1)}]^2[\gamma^{(2)}])$ $q\sigma \tilde{I}^{10} = \text{tr}([\gamma^{(1)}][\gamma^{(2)}]^2)$ ; $q\sigma \tilde{I}^{11} = \text{tr}([\gamma^{(1)}]^2[\gamma^{(2)}]^2)$
	(a) $\begin{cases} q\sigma \tilde{I} = \text{tr}([\gamma^{(1)}][\gamma^{(2)}] + [\gamma^{(2)}][\gamma^{(1)}]) \\ q\sigma \tilde{I} = \text{tr}([\gamma^{(1)}][\gamma^{(2)}] - [\gamma^{(2)}][\gamma^{(1)}]) \end{cases}$
$[\gamma^{(1)}]$ , $\bar{\mathbf{g}}$	$q\sigma \tilde{I}^{12} = \bar{\mathbf{g}} \cdot [\gamma^{(1)}] \bar{\mathbf{g}}$ ; $q\sigma \tilde{I}^{13} = \bar{\mathbf{g}} \cdot [\gamma^{(1)}]^2 \bar{\mathbf{g}}$
$[\gamma^{(2)}]$ , $\bar{\mathbf{g}}$	$q\sigma \tilde{I}^{14} = \bar{\mathbf{g}} \cdot [\gamma^{(2)}] \bar{\mathbf{g}}$ ; $q\sigma \tilde{I}^{15} = \bar{\mathbf{g}} \cdot [\gamma^{(2)}]^2 \bar{\mathbf{g}}$
(3) three at a time ( including (1) and(2) )	
$[\gamma^{(1)}]$ , $[\gamma^{(2)}]$ , $\bar{\mathbf{g}}$	$q\sigma \tilde{I}^{16} = \bar{\mathbf{g}} \cdot [\gamma^{(1)}][\gamma^{(2)}] \bar{\mathbf{g}}$
	(b) $\begin{cases} q\sigma \tilde{I} = \bar{\mathbf{g}} \cdot [\gamma^{(1)}][\gamma^{(2)}] + [\gamma^{(2)}][\gamma^{(1)}] \bar{\mathbf{g}} \\ q\sigma \tilde{I} = \bar{\mathbf{g}} \cdot [\gamma^{(1)}][\gamma^{(2)}] - [\gamma^{(2)}][\gamma^{(1)}] \bar{\mathbf{g}} \end{cases}$

Substituting 5.4 into 5.2 gives the most general form of the constitutive relations for  $[_{d\bar{\sigma}}^{(0)}]$  for thermoelastic compressible solids of order two in contra-variant basis. The final set of constants resulting in this expression for the constitutive equations for  $[_{d\bar{\sigma}}^{(0)}]$  must be determined experimentally.

### Co-variant basis

We express  $[_{d\bar{\sigma}}^{(1)}]$ , the first convected time derivative of the co-variant deviatoric Cauchy stress as a linear combinations of the combined generators of the argument tensors  $[\gamma_{(j)}]$  ;  $j = 1, 2, \dots, n$  and  $\bar{\mathbf{g}}$ . As in the contra-variant case, if we limit the kinematic tensors to just the first two, i.e.,  $[\gamma_{(1)}]$  and  $[\gamma_{(2)}]$ , then we have

$$[_{d\bar{\sigma}}^{(1)}] = [_{d\bar{\sigma}}^{(1)}](\bar{\rho}, [\gamma_{(1)}], [\gamma_{(2)}], \bar{\theta}, \bar{\mathbf{g}}) \quad (5.5)$$

We use 5.5 to present the remaining details. In this case we expect a total of twelve combined generators (as in the contra-variant case). Let us define these as  $[\sigma \tilde{G}_i]$  ;  $i = 1, 2, \dots, 12$ . These can be obtained using the definitions of  $[\sigma \tilde{G}^i]$  ;  $i = 1, 2, \dots, 12$  but replacing  $[\gamma^{(1)}]$  and  $[\gamma^{(2)}]$  with  $[\gamma_{(1)}]$  and  $[\gamma_{(2)}]$ . Likewise the

combined invariants  ${}^{q\sigma}\underline{I}_i ; i = 1, 2, \dots, 16$  can be obtained from  ${}^{q\sigma}\underline{I}^i ; i = 1, 2, \dots, 16$  by replacing  $[\gamma^{(1)}]$  and  $[\gamma^{(2)}]$  with  $[\gamma_{(1)}]$  and  $[\gamma_{(2)}]$ .

Now, we can express  $[{}_d\bar{\sigma}_{(1)}]$  as a linear combination of  $[I]$  and the combined generators  $[\sigma G_i] ; i = 1, 2, \dots, 12$  in the co-variant basis.

$$[{}_d\bar{\sigma}_{(1)}] = \sigma_{\alpha_0}[I] + \sum_{i=1}^{12} \sigma_{\alpha_i}[\sigma G_i] \quad (5.6)$$

The coefficients  $\sigma_{\alpha_i} ; i = 0, 1, \dots, 12$  are functions of the combined invariants  ${}^{q\sigma}\underline{I}_j ; j = 1, 2, \dots, 16, \bar{\rho}$  and  $\bar{\theta}$ . The coefficients  $\sigma_{\alpha_i} ; i = 0, 1, \dots, 12$  are determined by using the Taylor series expansion for each  $\sigma_{\alpha_i}$  about the reference configuration and only retaining up to linear terms in the combined invariants and  $\bar{\theta}$ .

$$\sigma_{\alpha_i} = \sigma_{\alpha_i} \Big|_{\text{ref}} + \sum_{j=1}^{16} \frac{\partial(\sigma_{\alpha_i})}{\partial({}^{q\sigma}\underline{I}_j)} \Big|_{\text{ref}} ({}^{q\sigma}\underline{I}_j - ({}^{q\sigma}\underline{I}_j)_0) + \frac{\partial(\sigma_{\alpha_i})}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 0, 1, \dots, 12 \quad (5.7)$$

in which the quantities with the subscript zero are their values in the reference configuration. Since  $({}^{q\sigma}\underline{I}_j)_0 ; j = 1, 2, \dots, 16$  are zero (for the same reasons as in the contra-variant case) and if  $\underline{\mathbf{g}}|_0 = 0$  then 5.7 reduces to

$$\sigma_{\alpha_i} = \sigma_{\alpha_i} \Big|_{\text{ref}} + \sum_{j=1}^{16} \frac{\partial(\sigma_{\alpha_i})}{\partial({}^{q\sigma}\underline{I}_j)} \Big|_{\text{ref}} {}^{q\sigma}\underline{I}_j + \frac{\partial(\sigma_{\alpha_i})}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 0, 1, \dots, 12 \quad (5.8)$$

By substituting from 5.8 into 5.6, we obtain the most general form of the constitutive equations for  $[{}_d\bar{\sigma}_{(1)}]$  (co-variant basis) for thermoelastic compressible solids of order two. Here also, the final set of constants resulting in this expression must be determined experimentally.

#### Remarks:

We have presented most general derivations of the constitutive theory for the deviatoric Cauchy stress tensor for ‘ordered thermoelastic compressible solids’ in contra- and co-variant bases with specific details for solids of order two. The derivations are made specific by choosing only first and second convected time derivatives of the Green’s strain and Almansi strain in co- and contra-variant bases to present details of the constitutive equations. Inclusion of the convected time derivatives of order higher than two as argument tensors poses no special problem except involving more and new combined generators and invariants. We make some important remarks in the following.

- (1) We note that  $[\gamma^{(j)}] \neq [\gamma_{(j)}] ; j = 2, 3, \dots, n$  and  $[{}_d\bar{\sigma}^{(1)}] \neq [{}_d\bar{\sigma}_{(1)}]$ . That is, the constitutive theory for deviatoric stress differs in contra- and co-variant bases.
- (2) In many practical applications involving thermoelastic compressible solids in Eulerian description the constitutive theory of order one is found to describe the physics adequately. In this case, the convected time derivative of order one of the chosen strain tensor will appear as argument tensor (in addition to density, temperature and temperature gradient) for all dependent variables in the constitutive theory giving rise to the constitutive equations for *thermoelastic compressible solids of order one*. In this case  $[{}_d\bar{\sigma}^{(1)}]$  is expressed as a linear combination of  $[I]$  and the combined generators of  $[\gamma^{(1)}]$  and  $\underline{\mathbf{g}}$  that are symmetric and are of rank two. The coefficients in the linear combination are functions of the combined invariants of  $[\gamma^{(1)}]$  and  $\underline{\mathbf{g}}$  (in addition to  $\bar{\rho}$  and  $\bar{\theta}$ ). By replacing  $[\gamma^{(1)}]$  with  $[\gamma_{(1)}]$  and  $[{}_d\bar{\sigma}^{(1)}]$  with  $[{}_d\bar{\sigma}_{(1)}]$  the contra-variant description can be converted to co-variant description for the deviatoric stress tensor. The details of the constitutive theory for this special case are presented in section 5.2.
- (3) Further simplifications of the constitutive theory described in remark (2) is also possible. For example, if we assume that the deviatoric stress only depends upon density, temperature and the first convected time derivative of the strain tensor (Green’s or Almansi depending upon co- or contra-variant basis), then we obtain a much simplified form of the constitutive equations for deviatoric stress in the chosen basis. From these constitutive equations we realize the well known relations for *generalized hypo-thermoelastic compressible solids*. The details of the constitutive equations for this special case are presented in section 5.3.

- (4) Upon further simplification of the constitutive theory described in remark (3) we obtain the well known constitutive equations for *hypo-thermoelastic compressible solids* for the deviatoric stress. These are obviously a subcategory of the general class of thermoelastic solids discussed in remark (2) (thermoelastic compressible solids of order one). The details of the constitutive equations described here are presented in section 5.4.

## 5.2 Thermoelastic solids of order one: compressible

We consider both contra- and co-variant basis.

### Contra-variant basis

In this case we have

$$[{}_d\bar{\sigma}^{(1)}] = [{}_d\bar{\sigma}^{(1)}(\bar{\rho}, [\gamma^{(1)}], \bar{\theta}, \bar{\mathbf{g}})] \quad (5.9)$$

$$\bar{\Phi} = \bar{\Phi}(\bar{\rho}, \bar{\theta}) \quad (5.10)$$

The combined generators of tensors  $[\gamma^{(1)}]$  and  $\bar{\mathbf{g}}$  are that are symmetric tensors of rank 2 are

$$[\sigma \tilde{G}^1] = [\gamma^{(1)}] \quad ; \quad [\sigma \tilde{G}^2] = [\gamma^{(1)}]^2 \quad ; \quad [\sigma \tilde{G}^3] = \bar{\mathbf{g}} \otimes \bar{\mathbf{g}} \quad (5.11)$$

The combined invariants of the tensors  $[\gamma^{(1)}]$  and  $\bar{\mathbf{g}}$  are

$$\begin{aligned} {}^{q\sigma}\tilde{I}^1 &= \text{tr}([\gamma^{(1)}]) \quad ; \quad {}^{q\sigma}\tilde{I}^2 = \text{tr}([\gamma^{(1)}]^2) \quad ; \quad {}^{q\sigma}\tilde{I}^3 = \text{tr}([\gamma^{(1)}]^3) \\ {}^{q\sigma}\tilde{I}^4 &= \bar{\mathbf{g}} \cdot \bar{\mathbf{g}} \quad ; \quad {}^{q\sigma}\tilde{I}^5 = \bar{\mathbf{g}} \cdot [\gamma^{(1)}] \bar{\mathbf{g}} \quad ; \quad {}^{q\sigma}\tilde{I}^6 = \bar{\mathbf{g}} \cdot [\gamma^{(1)}]^2 \bar{\mathbf{g}} \end{aligned} \quad (5.12)$$

$$\therefore \quad [{}_d\bar{\sigma}^{(1)}] = \sigma \hat{\alpha}^0 [I] + \sum_{i=1}^3 \sigma \hat{\alpha}^i [\sigma \tilde{G}^i] \quad (5.13)$$

The coefficients  $\sigma \hat{\alpha}^i$  are functions of  $\bar{\rho}$ ,  $\bar{\theta}$  and the combined invariants  ${}^{q\sigma}\tilde{I}^j$ ;  $j = 1, 2, \dots, 6$ . These are determined by using Taylor series expansion about the reference configuration and only retaining up to linear terms in the combined invariants and  $\bar{\theta}$ .

$$\sigma \hat{\alpha}^i = \sigma \hat{\alpha}^i \Big|_{\text{ref}} + \sum_{j=1}^6 \frac{\partial(\sigma \hat{\alpha}^i)}{\partial({}^{q\sigma}\tilde{I}^j)} \Big|_{\text{ref}} ({}^{q\sigma}\tilde{I}^j - ({}^{q\sigma}\tilde{I}^j)_0) + \frac{\partial(\sigma \hat{\alpha}^i)}{\partial \bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 0, 1, \dots, 3 \quad (5.14)$$

Since  $({}^{q\sigma}\tilde{I}^j)_0 = 0$ ;  $j = 1, 2, \dots, 6$ , expression 5.14 reduces to

$$\sigma \hat{\alpha}^i = \sigma \hat{\alpha}^i \Big|_{\text{ref}} + \sum_{j=1}^6 \frac{\partial(\sigma \hat{\alpha}^i)}{\partial({}^{q\sigma}\tilde{I}^j)} \Big|_{\text{ref}} {}^{q\sigma}\tilde{I}^j + \frac{\partial(\sigma \hat{\alpha}^i)}{\partial \bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 0, 1, \dots, 3 \quad (5.15)$$

By substituting from 5.15 into 5.13 we obtain the constitutive equations for  $[{}_d\bar{\sigma}^{(1)}]$ . This is the most general form of the constitutive theory for deviatoric stress for thermoelastic compressible solids of order one.

### Co-variant basis

In the co-variant case we have

$$[{}_d\bar{\sigma}_{(1)}] = [{}_d\bar{\sigma}_{(1)}(\bar{\rho}, [\gamma_{(1)}], \bar{\theta}, \bar{\mathbf{g}})] \quad (5.16)$$

$$\bar{\Phi} = \bar{\Phi}(\bar{\rho}, \bar{\theta}) \quad (5.17)$$

We note that  $[\gamma^{(1)}] = [\gamma_{(1)}]$ , i.e., the first convected time derivative of the Almansi strain in contra-variant basis is the same as the first convected time derivative of the Green's strain in the co-variant basis. Furthermore,  $\bar{\rho}$ ,  $\bar{\theta}$  and  $\bar{\mathbf{g}}$  are Eulerian descriptions involving coordinates  $\bar{x}_i$  of material points in the current configuration and hence are independent of co- and contra-variant description. But  $[{}_d\bar{\sigma}_{(1)}] \neq [{}_d\bar{\sigma}^{(1)}]$ . That is, the constitutive equations in the co- and contra-variant bases are not the same for thermoelastic solids of order one. The details of the derivation follows the contra-variant case and hence are omitted.

### 5.3 Generalized hypo-thermoelastic solids: compressible

If we remove the dependence of the convected time derivative of the stress tensor on  $\bar{\mathbf{g}}$ , we can derive a much simplified form of the constitutive theory. These are obviously a subcategory of the thermoelastic compressible solids of order one. These constitutive equations define hypo-thermoelastic compressible solid matter (similar to generalized Newtonian fluids [1]).

#### Contra-variant basis

In this case we have

$$[{}_d\bar{\sigma}^{(1)}] = [{}_d\bar{\sigma}^{(1)}(\bar{\rho}, [\gamma^{(1)}], \bar{\theta})] \quad (5.18)$$

$$\bar{\Phi} = \bar{\Phi}(\bar{\rho}, \bar{\theta}) \quad (5.19)$$

In this case the generators are only due to  $[\gamma^{(1)}]$

$$[\sigma \tilde{G}^1] = [\gamma^{(1)}] \quad ; \quad [\sigma \tilde{G}^2] = [\gamma^{(1)}]^2 \quad (5.20)$$

$$\therefore [{}_d\bar{\sigma}^{(1)}] = \sigma \tilde{\alpha}^0[I] + \sigma \tilde{\alpha}^1[\sigma \tilde{G}^1] + \sigma \tilde{\alpha}^2[\sigma \tilde{G}^2] \quad (5.21)$$

The invariants are also only due to  $[\gamma^{(1)}]$

$$\sigma \tilde{I}^1 = \text{tr}([\gamma^{(1)}]) \quad ; \quad \sigma \tilde{I}^2 = \text{tr}([\gamma^{(1)}]^2) \quad ; \quad \sigma \tilde{I}^3 = \text{tr}([\gamma^{(1)}]^3) \quad (5.22)$$

Hence  $\sigma \tilde{\alpha}^i$ ;  $i = 0, 1, 2$  are functions of  $\bar{\rho}, \bar{\theta}$  and  $\sigma \tilde{I}^j$ ;  $j = 1, 2, 3$ . Consider Taylor series expansion of  $\sigma \tilde{\alpha}^i$  about the reference configuration and retain only up to the linear terms in the invariants and  $\bar{\theta}$ .

$$\sigma \tilde{\alpha}^i = \sigma \tilde{\alpha}^i \Big|_{\text{ref}} + \sum_{j=1}^3 \frac{\partial(\sigma \tilde{\alpha}^i)}{\partial(\sigma \tilde{I}^j)} \Big|_{\text{ref}} (\sigma \tilde{I}^j - (\sigma \tilde{I}^j)_0) + \frac{\partial(\sigma \tilde{\alpha}^i)}{\partial \bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 0, 1, 2 \quad (5.23)$$

Since  $(\sigma \tilde{I}^j)_0 = 0$ ;  $j = 1, 2, 3$  due to the fact that  $[\gamma^{(1)}]_0 = 0$ , expression 5.23 reduces to

$$\sigma \tilde{\alpha}^i = \sigma \tilde{\alpha}^i \Big|_{\text{ref}} + \sum_{j=1}^3 \frac{\partial(\sigma \tilde{\alpha}^i)}{\partial(\sigma \tilde{I}^j)} \Big|_{\text{ref}} \sigma \tilde{I}^j + \frac{\partial(\sigma \tilde{\alpha}^i)}{\partial \bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 0, 1, 2 \quad (5.24)$$

If we let  $\frac{\partial(\sigma \tilde{\alpha}^i)}{\partial(\sigma \tilde{I}^j)} = \sigma \tilde{\alpha}^i_{,j}$ ;  $j = 1, 2, 3$ , then 5.24 becomes

$$\sigma \tilde{\alpha}^i = \sigma \tilde{\alpha}^i \Big|_{\text{ref}} + \sum_{j=1}^3 (\sigma \tilde{\alpha}^i_{,j})_0 \sigma \tilde{I}^j + \frac{\partial(\sigma \tilde{\alpha}^i)}{\partial \bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 0, 1, 2 \quad (5.25)$$

Substitution from 5.22 into 5.25 and then from 5.25 into 5.21

$$\begin{aligned} [{}_d\bar{\sigma}^{(1)}] = & \left( \sigma \tilde{\alpha}^0 \Big|_{\text{ref}} + (\sigma \tilde{\alpha}^0_{,1})_0 \text{tr}([\gamma^{(1)}]) + (\sigma \tilde{\alpha}^0_{,2})_0 \text{tr}([\gamma^{(1)}]^2) + (\sigma \tilde{\alpha}^0_{,3})_0 \text{tr}([\gamma^{(1)}]^3) + \frac{\partial(\sigma \tilde{\alpha}^0)}{\partial \bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \right) [I] \\ & \left( \sigma \tilde{\alpha}^1 \Big|_{\text{ref}} + (\sigma \tilde{\alpha}^1_{,1})_0 \text{tr}([\gamma^{(1)}]) + (\sigma \tilde{\alpha}^1_{,2})_0 \text{tr}([\gamma^{(1)}]^2) + (\sigma \tilde{\alpha}^1_{,3})_0 \text{tr}([\gamma^{(1)}]^3) + \frac{\partial(\sigma \tilde{\alpha}^1)}{\partial \bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \right) [\gamma^{(1)}] \\ & \left( \sigma \tilde{\alpha}^2 \Big|_{\text{ref}} + (\sigma \tilde{\alpha}^2_{,1})_0 \text{tr}([\gamma^{(1)}]) + (\sigma \tilde{\alpha}^2_{,2})_0 \text{tr}([\gamma^{(1)}]^2) + (\sigma \tilde{\alpha}^2_{,3})_0 \text{tr}([\gamma^{(1)}]^3) + \frac{\partial(\sigma \tilde{\alpha}^2)}{\partial \bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \right) [\gamma^{(1)}]^2 \end{aligned} \quad (5.26)$$

Collecting coefficients and defining  $\tilde{\theta} = \bar{\theta} - \theta_0$ , 5.26 can be written as

$$[{}_d\bar{\sigma}^{(1)}] = \sigma \tilde{\alpha}^0 \Big|_{\text{ref}} \left[ I + \frac{\partial(\sigma \tilde{\alpha}^0)}{\partial \bar{\theta}} \Big|_{\text{ref}} \tilde{\theta} \right] + \sigma b(\bar{\rho}, [\gamma^{(1)}], \tilde{\theta}) [I] + \sigma b^1(\bar{\rho}, [\gamma^{(1)}], \tilde{\theta}) [\gamma^{(1)}] + \sigma b^2(\bar{\rho}, [\gamma^{(1)}], \tilde{\theta}) [\gamma^{(1)}]^2 \quad (5.27)$$

where

$$\begin{aligned}\sigma b(\bar{\rho}, [\gamma^{(1)}], \bar{\theta}) &= (\sigma \tilde{\alpha}^0, 1)_0 \text{tr}([\gamma^{(1)}]) + (\sigma \tilde{\alpha}^0, 2)_0 \text{tr}([\gamma^{(1)}]^2) + (\sigma \tilde{\alpha}^0, 3)_0 \text{tr}([\gamma^{(1)}]^3) \\ \sigma b^1(\bar{\rho}, [\gamma^{(1)}], \bar{\theta}) &= \sigma \tilde{\alpha}^1 \Big|_{\text{ref}} + (\sigma \tilde{\alpha}^1, 1)_0 \text{tr}([\gamma^{(1)}]) + (\sigma \tilde{\alpha}^1, 2)_0 \text{tr}([\gamma^{(1)}]^2) + (\sigma \tilde{\alpha}^1, 3)_0 \text{tr}([\gamma^{(1)}]^3) + \frac{\partial(\sigma \tilde{\alpha}^1)}{\partial \bar{\theta}} \Big|_{\text{ref}} \bar{\theta} \\ \sigma b^2(\bar{\rho}, [\gamma^{(1)}], \bar{\theta}) &= \sigma \tilde{\alpha}^2 \Big|_{\text{ref}} + (\sigma \tilde{\alpha}^2, 1)_0 \text{tr}([\gamma^{(1)}]) + (\sigma \tilde{\alpha}^2, 2)_0 \text{tr}([\gamma^{(1)}]^2) + (\sigma \tilde{\alpha}^2, 3)_0 \text{tr}([\gamma^{(1)}]^3) + \frac{\partial(\sigma \tilde{\alpha}^2)}{\partial \bar{\theta}} \Big|_{\text{ref}} \bar{\theta}\end{aligned}\quad (5.28)$$

Equation 5.27 is the final form of the constitutive equations based on argument tensors in 5.18. We note that 5.27 is quadratic in  $[\gamma^{(1)}]$ , i.e., it has generators  $[\gamma^{(1)}]$  and  $[\gamma^{(1)}]^2$ . The coefficients  $\sigma b$ ,  $\sigma b^1$  and  $\sigma b^2$  are functions of the invariants of the strain rate tensor  $[\gamma^{(1)}]$ , density  $\bar{\rho}$  and temperature  $\bar{\theta}$ . The first term on the right side of equation 5.27 describes the initial stress field in the reference configuration. The second terms account for the stress field in the current configuration due to temperature change.

### Co-variant basis

In the co-variant case we have

$$[{}_d\bar{\sigma}_{(1)}] = [{}_d\bar{\sigma}_{(1)}(\bar{\rho}, [\gamma^{(1)}], \bar{\theta})] \quad (5.29)$$

$$\bar{\Phi} = \bar{\Phi}(\bar{\rho}, \bar{\theta}) \quad (5.30)$$

The derivation is parallel to the contra-variant case except that  $[{}_d\bar{\sigma}_{(1)}]$  replaces  $[{}_d\bar{\sigma}^{(1)}]$  and  $[\gamma^{(1)}]$  replaces  $[\gamma^{(1)}]$ . Details are omitted.

## 5.4 Hypo-thermoelastic solids: compressible

In this section we discuss further assumptions and simplifications of the constitutive theory of generalized hypo-thermoelastic compressible solids.

### Contra-variant basis

If we assume that  $[{}_d\bar{\sigma}^{(1)}]$  only depends on the generator  $[\gamma^{(1)}]$ , then 5.27 reduces to

$$[{}_d\bar{\sigma}^{(1)}] = \sigma \tilde{\alpha}^0 \Big|_{\text{ref}} [I] + \frac{\partial(\sigma \tilde{\alpha}^0)}{\partial \bar{\theta}} \Big|_{\text{ref}} \bar{\theta} [I] + \sigma b(\bar{\rho}, [\gamma^{(1)}], \bar{\theta}) [I] + \sigma b^1(\bar{\rho}, [\gamma^{(1)}], \bar{\theta}) [\gamma^{(1)}] \quad (5.31)$$

The constitutive equation 5.31 describes restricted generalized hypo-thermoelastic compressible solids.

Equation 5.31 can be further simplified if we neglect the infinitesimals of orders two and higher in the velocity gradients appearing in  $[\gamma^{(1)}]$  and its invariants.

$$[{}_d\bar{\sigma}^{(1)}] = \sigma \tilde{\alpha}^0 \Big|_{\text{ref}} [I] + \frac{\partial(\sigma \tilde{\alpha}^0)}{\partial \bar{\theta}} \Big|_{\text{ref}} \bar{\theta} [I] + (\sigma \tilde{\alpha}^0, 1)_0 \text{tr}([\gamma^{(1)}]) [I] + \sigma \tilde{\alpha}^1 \Big|_{\text{ref}} [\gamma^{(1)}] \quad (5.32)$$

Let us define

$$\kappa(\bar{\rho}, \bar{\theta}) = (\sigma \tilde{\alpha}^0, 1)_0 \quad ; \quad 2\mu(\bar{\rho}, \bar{\theta}) = \sigma \tilde{\alpha}^1 \Big|_{\text{ref}} \quad (5.33)$$

Then 5.32 becomes

$$[{}_d\bar{\sigma}^{(1)}] = \sigma \tilde{\alpha}^0 \Big|_{\text{ref}} [I] + \frac{\partial(\sigma \tilde{\alpha}^0)}{\partial \bar{\theta}} \Big|_{\text{ref}} \bar{\theta} [I] + \kappa(\bar{\rho}, \bar{\theta}) \text{tr}([\gamma^{(1)}]) [I] + 2\mu(\bar{\rho}, \bar{\theta}) [\gamma^{(1)}] \quad (5.34)$$

This is the constitutive equation for hypo-thermoelastic compressible solids. If the reference configuration is stress free and if the stress field due to expansion and contraction are neglected then 5.34 reduces to

$$[{}_d\bar{\sigma}^{(1)}] = 2\mu(\bar{\rho}, \bar{\theta}) [\gamma^{(1)}] + \kappa(\bar{\rho}, \bar{\theta}) \text{tr}([\gamma^{(1)}]) [I] \quad (5.35)$$

which is the standard constitutive equation for hypo-thermoelastic compressible solids;  $\mu$  is shear modulus and  $\kappa$  is the bulk modulus.

### Co-variant basis

In this case we have

$$[{}_d\bar{\sigma}_{(1)}] = [{}_d\bar{\sigma}_{(1)}(\bar{\rho}, [\gamma_{(1)}], \bar{\theta})] \quad (5.36)$$

$$\bar{\Phi} = \bar{\Phi}(\bar{\rho}, \bar{\theta}) \quad (5.37)$$

The derivation is parallel to the contra-variant case except that  $[{}_d\bar{\sigma}_{(1)}]$  replaces  $[{}_d\bar{\sigma}^{(1)}]$  and  $[\gamma_{(1)}]$  replaces  $[\gamma^{(1)}]$ . Details are omitted.

## 6 Development of the constitutive equations for the deviatoric Cauchy stress tensor: incompressible

The derivations presented in section 5 hold for compressible ordered thermoelastic solids. In this section we consider the incompressible case. In the case of incompressible matter we have

$$\text{div}(\mathbf{v}) = 0 \quad (6.1)$$

due to continuity equation which implies that

$$\text{tr}([\gamma^{(1)}]) = \text{tr}([\gamma_{(1)}]) = \text{tr}([\gamma^{(0)}]) = \text{tr}([\gamma_{(0)}]) = 0 \quad (6.2)$$

or alternatively, since  $\bar{\rho} = \rho = \text{constant}$ , then the following must hold for incompressible matter.

$$\det[J] = 1 \quad (6.3)$$

### 6.1 Most general form of the constitutive equations for the deviatoric stress tensor

The general theory and the constitutive equations for compressible thermoelastic solids of order two and one presented in section 5 can be easily modified by incorporating the incompressibility assumptions 6.1 - 6.3. This is straight forward and hence the details are omitted. The constitutive equations presented in section 5 for compressible generalized hypo-thermoelastic solids and compressible hypo-thermoelastic solids are used to derive the constitutive equations for the incompressible case in the following.

### 6.2 Generalized hypo-thermoelastic solids: incompressible

In this case 5.18 and 5.19 reduce to (using contra-variant basis)

$$[{}_d\bar{\sigma}^{(1)}] = [{}_d\bar{\sigma}^{(1)}([\gamma^{(1)}], \bar{\theta})] \quad (6.4)$$

$$\bar{\Phi} = \bar{\Phi}(\bar{\theta}) \quad (6.5)$$

with the incompressibility condition

$$\sigma \tilde{I}^1 = \text{tr}([\gamma^{(1)}]) = 0 \quad (6.6)$$

Hence, following the derivation in section 5.3, we can obtain 5.27 in which the coefficients  $\sigma b$ ,  $\sigma b^1$  and  $\sigma b^2$  must be modified using 6.6. If we assume that  $[{}_d\bar{\sigma}^{(0)}]$  only depends on the generator  $[\gamma^{(1)}]$ , then 5.27 reduces to 5.31 in which  $\sigma b$  and  $\sigma b^1$  are modified to account for incompressibility. We present details in the following.

$$[{}_d\bar{\sigma}^{(1)}] = \sigma \tilde{\alpha}^0 \Big|_{\text{ref}} [I] + \frac{\partial(\sigma \tilde{\alpha}^0)}{\partial \bar{\theta}} \Big|_{\text{ref}} \tilde{\theta} [I] + \sigma b([\gamma^{(1)}], \bar{\theta}) [I] + \sigma b^1([\gamma^{(1)}], \bar{\theta}) [\gamma^{(1)}] \quad (6.7)$$

in which

$$\begin{aligned} \sigma b([\gamma^{(1)}], \bar{\theta}) &= (\sigma \tilde{\alpha}^0, 2)_0 \text{tr}([\gamma^{(1)}]^2) + (\sigma \tilde{\alpha}^0, 3)_0 \text{tr}([\gamma^{(1)}]^3) \\ \sigma b^1([\gamma^{(1)}], \bar{\theta}) &= \sigma \tilde{\alpha}^1 \Big|_{\text{ref}} + (\sigma \tilde{\alpha}^1, 2)_0 \text{tr}([\gamma^{(1)}]^2) + (\sigma \tilde{\alpha}^1, 3)_0 \text{tr}([\gamma^{(1)}]^3) + \frac{\partial(\sigma \tilde{\alpha}^1)}{\partial \bar{\theta}} \Big|_{\text{ref}} \tilde{\theta} \end{aligned} \quad (6.8)$$

These describe the most general form of a generalized hypo-thermoelastic incompressible solid based on 6.4 - 6.6.

### 6.3 Hypo-thermoelastic solids: incompressible

If we neglect infinitesimals of order three in the components of  $[\gamma^{(1)}]$ , then we can neglect the terms containing  $\text{tr}([\gamma^{(1)}]^3)$  in 6.8 which results in modification of the coefficients  $\sigma b$ ,  $\sigma b^1$  giving

$$\begin{aligned}\sigma b([\gamma^{(1)}], \bar{\theta}) &= (\sigma \tilde{\alpha}^0, 2)_0 \text{tr}([\gamma^{(1)}]^2) \\ \sigma b^1([\gamma^{(1)}], \bar{\theta}) &= \sigma \tilde{\alpha}^1 \Big|_{\text{ref}} + (\sigma \tilde{\alpha}^1, 2)_0 \text{tr}([\gamma^{(1)}]^2) + \frac{\partial(\sigma \tilde{\alpha}^1)}{\partial \bar{\theta}} \Big|_{\text{ref}} \tilde{\theta}\end{aligned}\quad (6.9)$$

Substituting 6.9 into 6.7

$$\begin{aligned}[_d \bar{\sigma}^{(1)}] &= \sigma \tilde{\alpha}^0 \Big|_{\text{ref}} [I] + \frac{\partial(\sigma \tilde{\alpha}^0)}{\partial \bar{\theta}} \Big|_{\text{ref}} \tilde{\theta} [I] + ((\sigma \tilde{\alpha}^0, 2)_0 \text{tr}([\gamma^{(1)}]^2)) [I] \\ &\quad + (\sigma \tilde{\alpha}^1 \Big|_{\text{ref}} + (\sigma \tilde{\alpha}^1, 2)_0 \text{tr}([\gamma^{(1)}]^2) + \frac{\partial(\sigma \tilde{\alpha}^1)}{\partial \bar{\theta}} \Big|_{\text{ref}} \tilde{\theta}) [\gamma^{(1)}]\end{aligned}\quad (6.10)$$

which can be written as

$$\begin{aligned}[_d \bar{\sigma}^{(1)}] &= \sigma \tilde{\alpha}^0 \Big|_{\text{ref}} [I] + \frac{\partial(\sigma \tilde{\alpha}^0)}{\partial \bar{\theta}} \Big|_{\text{ref}} \tilde{\theta} [I] + \sigma \tilde{\alpha}^1 \Big|_{\text{ref}} [\gamma^{(1)}] + ((\sigma \tilde{\alpha}^0, 2)_0 \text{tr}([\gamma^{(1)}]^2)) [I] \\ &\quad + ((\sigma \tilde{\alpha}^1, 2)_0 \text{tr}([\gamma^{(1)}]^2) + \frac{\partial(\sigma \tilde{\alpha}^1)}{\partial \bar{\theta}} \Big|_{\text{ref}} \tilde{\theta}) [\gamma^{(1)}]\end{aligned}\quad (6.11)$$

Equation 6.11 is the simplified form for the generalized hypo-thermoelastic incompressible solid matter. If we define

$$\begin{aligned}2\mu(\bar{\theta}) &= \sigma \tilde{\alpha}^1 \Big|_{\text{ref}} \\ \eta_1(\text{tr}([\gamma^{(1)}]^2), \bar{\theta}) &= (\sigma \tilde{\alpha}^0, 2)_0 \text{tr}([\gamma^{(1)}]^2) \\ \eta_2(\text{tr}([\gamma^{(1)}]^2), \bar{\theta}) &= (\sigma \tilde{\alpha}^1, 2)_0 \text{tr}([\gamma^{(1)}]^2) + \frac{\partial(\sigma \tilde{\alpha}^1)}{\partial \bar{\theta}} \Big|_{\text{ref}} \tilde{\theta}\end{aligned}\quad (6.12)$$

Then 6.11 can be written as

$$[_d \bar{\sigma}^{(1)}] = \sigma \tilde{\alpha}^0 \Big|_{\text{ref}} [I] + \frac{\partial(\sigma \tilde{\alpha}^0)}{\partial \bar{\theta}} \Big|_{\text{ref}} \tilde{\theta} [I] + 2\mu(\bar{\theta}) [\gamma^{(1)}] + \eta_1(\text{tr}([\gamma^{(1)}]^2), \bar{\theta}) [I] + \eta_2(\text{tr}([\gamma^{(1)}]^2), \bar{\theta}) [\gamma^{(1)}] \quad (6.13)$$

where  $\mu(\bar{\theta})$  is the shear modulus,  $\eta_1$  and  $\eta_2$  are coefficients dependent on the second invariant of  $[\gamma^{(1)}]$  and the temperature  $\bar{\theta}$  in the current configuration. At this point we remark that none of the constitutive equations for  $[_d \bar{\sigma}^{(0)}]$  presented here for generalized hypo-thermoelastic solid matter are parallel to generalized Newtonian fluids [1]. In 6.13 if we neglect infinitesimals of order two of the components of  $[\gamma^{(1)}]$ , i.e., neglect  $(\text{tr}([\gamma^{(1)}]^2))$  terms, then 6.13 reduces to

$$[_d \bar{\sigma}^{(1)}] = \sigma \tilde{\alpha}^0 \Big|_{\text{ref}} [I] + \frac{\partial(\sigma \tilde{\alpha}^0)}{\partial \bar{\theta}} \Big|_{\text{ref}} \tilde{\theta} [I] + 2\mu(\bar{\theta}) [\gamma^{(1)}] \quad (6.14)$$

If we assume the reference configuration to be stress free and if we neglect the thermal expansion or contraction, then 6.14 reduces to

$$[_d \bar{\sigma}^{(1)}] = 2\mu(\bar{\theta}) [\gamma^{(1)}] \quad (6.15)$$

The constitutive equations 6.14 and 6.15 describe hypo-thermoelastic incompressible solids in which  $\mu(\bar{\theta})$  is temperature dependent shear modulus.

**Remarks:**

- (1) The constitutive equation in co-variant basis for  $[d\bar{\sigma}_{(1)}]$  can be easily obtained by replacing  $[\gamma^{(i)}]$  with  $[\gamma_{(i)}]$ ;  $i = 1, 2, \dots, n$  in the derivations presented for the contra-variant basis.
- (2) Temperature dependent shear modulus, i.e.,  $\mu(\bar{\theta})$  and also  $\eta_1(\bar{\theta})$ ,  $\eta_2(\bar{\theta})$  are valid. Thus Sutherland's law and power law for temperature dependent  $\mu$ ,  $\eta_1$ ,  $\eta_2$  are valid as long as their values are positive.

## 7 Constitutive equation for the heat vector: compressible

In this section we consider the most general case as well as some specific cases in which we limit the number of argument tensors  $[\gamma^{(j)}]$  or  $[\gamma_{(j)}]$ ;  $j = 1, 2, \dots, n$  to  $[\gamma^{(1)}]$  and  $[\gamma^{(2)}]$  for the constitutive equation for the heat vector.

### 7.1 Thermoelastic solids of order two: compressible

#### Contra-variant basis

In contra-variant basis, the general form of the heat vector is

$$\bar{\mathbf{q}}^{(0)} = \bar{\mathbf{q}}^{(0)}(\bar{\rho}, [\gamma^{(j)}]; j = 1, 2, \dots, n, \bar{\theta}, \bar{\mathbf{g}}) \quad (7.1)$$

Since  $\bar{\mathbf{q}}^{(0)}$  is a tensor of rank one, we need combined generators of  $[\gamma^{(j)}]$ ;  $j = 1, 2, \dots, n$  (tensors of rank two) and  $\bar{\mathbf{g}}$  (tensor of rank one) that are of rank one [16, 17, 19–29]. In the derivation presented in the following, we limit the argument tensors  $[\gamma^{(j)}]$ ;  $j = 1, 2, \dots, n$  to just two, i.e., we only consider  $[\gamma^{(1)}]$  and  $[\gamma^{(2)}]$  (extension to more arguments presents no difficulty except that the details become more involved). Thus we have

$$\bar{\mathbf{q}}^{(0)} = \bar{\mathbf{q}}^{(0)}(\bar{\rho}, [\gamma^{(1)}], [\gamma^{(2)}], \bar{\theta}, \bar{\mathbf{g}}) \quad (7.2)$$

Table 3.3 lists combined generators for  $\bar{\mathbf{q}}^{(0)}$ . The combined invariants remain the same as for  $[d\bar{\sigma}^{(0)}]$  which are listed in table 3.2. Now we can express  $\bar{\mathbf{q}}^{(0)}$  as a linear combination of the combined generators  $\{\tilde{q}^i G^i\}$ ;  $i = 1, 2, \dots, 7$  in the contra-variant basis.

$$\bar{\mathbf{q}}^{(0)} = - \sum_{i=1}^7 q_{\alpha^i} \{\tilde{q}^i G^i\} \quad (7.3)$$

The coefficients  $q_{\alpha^i}$ ;  $i = 1, 2, \dots, 7$  are functions of the combined invariants  ${}^{q\sigma} \tilde{I}^j$ ;  $j = 1, 2, \dots, 16$ , density  $\bar{\rho}$  and temperature  $\bar{\theta}$ . The coefficients  $q_{\alpha^i}$ ;  $i = 1, 2, \dots, 7$  are determined by using Taylor series expansion for each  $q_{\alpha^i}$  about the reference configuration and retaining only up to linear terms in the combined invariants and  $\bar{\theta}$ .

$$q_{\alpha^i} = q_{\alpha^i} \Big|_{\text{ref}} + \sum_{j=1}^{16} \frac{\partial(q_{\alpha^i})}{\partial({}^{q\sigma} \tilde{I}^j)} \Big|_{\text{ref}} ({}^{q\sigma} \tilde{I}^j - ({}^{q\sigma} \tilde{I}^j)_0) + \frac{\partial(q_{\alpha^i})}{\partial \bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 1, 2, \dots, 7 \quad (7.4)$$

in which the quantities with the subscript zero are their values in the reference configuration. As before,  $({}^{q\sigma} \tilde{I}^j)_0$ ;  $j = 1, 2, \dots, 16$  are all zero, and if  $\bar{\mathbf{g}}|_0 = 0$ , then 7.4 reduces to

$$q_{\alpha^i} = q_{\alpha^i} \Big|_{\text{ref}} + \sum_{j=1}^{16} \frac{\partial(q_{\alpha^i})}{\partial({}^{q\sigma} \tilde{I}^j)} \Big|_{\text{ref}} {}^{q\sigma} \tilde{I}^j + \frac{\partial(q_{\alpha^i})}{\partial \bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 1, 2, \dots, 7 \quad (7.5)$$

Substituting 7.5 in 7.3 gives the most general form of the constitutive equation for the heat vector  $\bar{\mathbf{q}}^{(0)}$  for ordered thermoelastic compressible solids of order two in contra-variant basis. The final set of constants (or coefficients) appearing in the constitutive equation for  $\bar{\mathbf{q}}^{(0)}$  must be determined experimentally.

Table 3.3: Combined generators for  $\bar{\mathbf{q}}^{(0)}$ 

Arguments	Generators
(1) one at a time	
$[\gamma^{(1)}]$	none
$[\gamma^{(2)}]$	none
$\bar{\mathbf{g}}$	$\{^q\widetilde{G}^1\} = \bar{\mathbf{g}}$
(2) two at a time ( including (1) )	
$[\gamma^{(1)}]$ , $[\gamma^{(2)}]$	none
$[\gamma^{(1)}]$ , $\bar{\mathbf{g}}$	$\{^q\widetilde{G}^2\} = [\gamma^{(1)}] \bar{\mathbf{g}}$ $\{^q\widetilde{G}^3\} = [\gamma^{(1)}]^2 \bar{\mathbf{g}}$
$[\gamma^{(2)}]$ , $\bar{\mathbf{g}}$	$\{^q\widetilde{G}^4\} = [\gamma^{(2)}] \bar{\mathbf{g}}$ $\{^q\widetilde{G}^5\} = [\gamma^{(2)}]^2 \bar{\mathbf{g}}$
(3) three at a time ( including (1) and (2) )	
$[\gamma^{(1)}]$ , $[\gamma^{(2)}]$ , $\bar{\mathbf{g}}$	$\{^q\widetilde{G}^6\} = [[\gamma^{(1)}][\gamma^{(2)}] + [\gamma^{(2)}][\gamma^{(1)}]] \bar{\mathbf{g}}$ $\{^q\widetilde{G}^7\} = [[\gamma^{(1)}][\gamma^{(2)}] - [\gamma^{(2)}][\gamma^{(1)}]] \bar{\mathbf{g}}$

### Co-variant basis

In co-variant basis we have

$$\bar{\mathbf{q}}_{(0)} = \bar{\mathbf{q}}_{(0)}(\bar{\rho}, [\gamma_{(j)}]; j = 1, 2, \dots, n, \bar{\theta}, \bar{\mathbf{g}}) \quad (7.6)$$

As in the the case of contra-variant basis, here also, if we limit the fundamental kinematic tensors  $[\gamma_{(j)}]$  to just  $[\gamma_{(1)}]$  and  $[\gamma_{(2)}]$  then we have

$$\bar{\mathbf{q}}_{(0)} = \bar{\mathbf{q}}_{(0)}(\bar{\rho}, [\gamma_{(1)}], [\gamma_{(2)}], \bar{\theta}, \bar{\mathbf{g}}) \quad (7.7)$$

In this case also (as in contra-variant basis) we have seven combined generators  $\{^q\widetilde{G}_i\}; i = 1, 2, \dots, 7$  and the combined invariants remain the same as for  $[_d\bar{\sigma}_{(0)}]$ , i.e., same as  $^q\sigma I_i; i = 1, 2, \dots, 16$ . The combined generators  $\{^q\widetilde{G}_i\}; i = 1, 2, \dots, 7$  can be obtained from  $\{^q\widetilde{G}^i\}; i = 1, 2, \dots, 7$  by replacing  $[\gamma^{(1)}]$  and  $[\gamma^{(2)}]$  with  $[\gamma_{(1)}]$  and  $[\gamma_{(2)}]$ . Now we can express  $\bar{\mathbf{q}}_{(0)}$  as

$$\bar{\mathbf{q}}_{(0)} = - \sum_{i=1}^7 q_{\alpha_i} \{^q\widetilde{G}_i\} \quad (7.8)$$

The coefficients  $q_{\alpha_i}; i = 1, 2, \dots, 7$  are functions of the combined invariants  $^q\sigma I_i; i = 1, 2, \dots, 16$ , density  $\bar{\rho}$  and temperature  $\bar{\theta}$ . The coefficients  $q_{\alpha_i}$  are determined by using Taylor series expansion for each  $q_{\alpha_i}$  about the

reference configuration and retaining only up to linear terms in the combined invariants and  $\bar{\theta}$ .

$${}^q\alpha_i = {}^q\alpha_i \Big|_{\text{ref}} + \sum_{j=1}^{16} \frac{\partial({}^q\alpha_i)}{\partial({}^{q\sigma}\underline{I}_j)} \Big|_{\text{ref}} ({}^{q\sigma}\underline{I}_j - ({}^{q\sigma}\underline{I}_j)_0) + \frac{\partial({}^q\alpha_i)}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 1, 2, \dots, 7 \quad (7.9)$$

As before, the quantities with the subscript zero are their values in the reference configuration and  $({}^{q\sigma}\underline{I}_j)_0$  ;  $j = 1, 2, \dots, 16$  are all zero (for the same reasons as before) and if  $\bar{\mathbf{g}}|_0 = 0$  then 7.9 can be written as

$${}^q\alpha_i = {}^q\alpha_i \Big|_{\text{ref}} + \sum_{j=1}^{16} \frac{\partial({}^q\alpha_i)}{\partial({}^{q\sigma}\underline{I}_j)} \Big|_{\text{ref}} {}^{q\sigma}\underline{I}_j + \frac{\partial({}^q\alpha_i)}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 1, 2, \dots, 7 \quad (7.10)$$

Substituting from 7.10 into 7.8 gives the most general form of constitutive equations for the heat vector  $\bar{\mathbf{q}}_{(0)}$  for ordered thermoelastic compressible solids of order two in co-variant basis. Determination of the constants (or coefficients) in this final form must be done experimentally.

## 7.2 Thermoelastic solids of order one: compressible

### Contra-variant basis

In contra-variant basis we have

$$\bar{\mathbf{q}}^{(0)} = \bar{\mathbf{q}}^{(0)}(\bar{\rho}, [\gamma^{(1)}], \bar{\theta}, \bar{\mathbf{g}}) \quad (7.11)$$

The combined generators of the tensors  $[\gamma^{(1)}]$  and  $\bar{\mathbf{g}}$  that are of rank one are

$$\{ {}^q\tilde{G}^1 \} = \bar{\mathbf{g}} \quad ; \quad \{ {}^q\tilde{G}^2 \} = [\gamma^{(1)}] \bar{\mathbf{g}} \quad ; \quad \{ {}^q\tilde{G}^3 \} = [\gamma^{(1)}]^2 \bar{\mathbf{g}} \quad (7.12)$$

The combined invariants of the tensors  $[\gamma^{(1)}]$  and  $\bar{\mathbf{g}}$  are given by

$$\begin{aligned} {}^{q\sigma}\tilde{I}^1 &= \text{tr}([\gamma^{(1)}]) \quad ; \quad {}^{q\sigma}\tilde{I}^2 = \text{tr}([\gamma^{(1)}]^2) \quad ; \quad {}^{q\sigma}\tilde{I}^3 = \text{tr}([\gamma^{(1)}]^3) \\ {}^{q\sigma}\tilde{I}^4 &= \bar{\mathbf{g}} \cdot \bar{\mathbf{g}} \quad ; \quad {}^{q\sigma}\tilde{I}^5 = \bar{\mathbf{g}} \cdot [\gamma^{(1)}] \bar{\mathbf{g}} \quad ; \quad {}^{q\sigma}\tilde{I}^6 = \bar{\mathbf{g}} \cdot [\gamma^{(1)}]^2 \bar{\mathbf{g}} \end{aligned} \quad (7.13)$$

$$\therefore \quad \bar{\mathbf{q}}^{(0)} = - \sum_{i=1}^3 {}^q\hat{\alpha}^i \{ {}^q\tilde{G}^i \} \quad (7.14)$$

The coefficients  ${}^q\hat{\alpha}^i$  are functions of  $\bar{\rho}$ ,  $\bar{\theta}$  and the invariants  ${}^{q\sigma}\tilde{I}^j$  ;  $j = 1, 2, \dots, 6$  given by 7.13. These are determined by using Taylor series expansion about the reference configuration and only retaining up to linear terms in the combined invariants and  $\bar{\theta}$ .

$${}^q\hat{\alpha}^i = {}^q\hat{\alpha}^i \Big|_{\text{ref}} + \sum_{j=1}^6 \frac{\partial({}^q\hat{\alpha}^i)}{\partial({}^{q\sigma}\tilde{I}^j)} \Big|_{\text{ref}} ({}^{q\sigma}\tilde{I}^j - ({}^{q\sigma}\tilde{I}^j)_0) + \frac{\partial({}^q\hat{\alpha}^i)}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 0, 1, \dots, 3 \quad (7.15)$$

Since  $({}^{q\sigma}\tilde{I}^j)_0 = 0$  ;  $j = 1, 2, \dots, 6$ , expression 7.15 reduces to

$${}^q\hat{\alpha}^i = {}^q\hat{\alpha}^i \Big|_{\text{ref}} + \sum_{j=1}^6 \frac{\partial({}^q\hat{\alpha}^i)}{\partial({}^{q\sigma}\tilde{I}^j)} \Big|_{\text{ref}} {}^{q\sigma}\tilde{I}^j + \frac{\partial({}^q\hat{\alpha}^i)}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 0, 1, \dots, 3 \quad (7.16)$$

By substituting from 7.16 into 7.14 we obtain the final form of the constitutive equation for the heat vector  $\bar{\mathbf{q}}^{(0)}$ . This is the most general form of the constitutive equation for the heat vector for thermoelastic compressible solids of order one.

### Co-variant basis

In co-variant basis we have

$$\bar{\mathbf{q}}_{(0)} = \bar{\mathbf{q}}_{(0)}(\bar{\rho}, [\gamma_{(1)}], \bar{\theta}, \bar{\mathbf{g}}) \quad (7.17)$$

We note that  $[\gamma^{(1)}] = [\gamma_{(1)}]$ , i.e., the first convected time derivative of the Almansi strain in contra-variant basis is the same as the first convected time derivative of the Green's strain in the co-variant basis. Furthermore,  $\bar{\rho}$ ,  $\bar{\theta}$  and  $\bar{\mathbf{g}}$  are in Eulerian description involving coordinates  $\bar{x}_i$  of material points in the current configuration and hence are independent of co- and contra-variant description. Hence, it is straight forward to conclude that  $\bar{\mathbf{q}}^{(0)} = \bar{\mathbf{q}}_{(0)}$ , i.e., for thermoelastic compressible solids of order one, the constitutive equations in the co- and contra-variant bases for the heat vector are identical.

### 7.3 Generalized hypo-thermoelastic solids: compressible

#### Contra-variant basis

In this case we do not consider dependence of  $\bar{\mathbf{q}}_{(0)}$  on  $[\gamma^{(j)}]$ , i.e.

$$\bar{\mathbf{q}}^{(0)} = \bar{\mathbf{q}}^{(0)}(\bar{\rho}, \bar{\theta}, \bar{\mathbf{g}}) \quad (7.18)$$

and the only generator is  $\bar{\mathbf{g}}$ , hence we can write

$$\bar{\mathbf{q}}^{(0)} = -{}^q\tilde{\alpha} \bar{\mathbf{g}} \quad (7.19)$$

Also, in this case the only invariant is  $\tilde{I}^1 = \bar{\mathbf{g}} \cdot \bar{\mathbf{g}}$ . Thus  ${}^q\tilde{\alpha}$  is a function of  $\tilde{I}^1$  and  $\bar{\theta}$ . Expanding  ${}^q\tilde{\alpha}$  in Taylor series about the reference configuration and retaining only up to linear terms in the invariant and  $\bar{\theta}$

$${}^q\tilde{\alpha} = {}^q\tilde{\alpha} \Big|_{\text{ref}} + \frac{\partial({}^q\tilde{\alpha})}{\partial(\tilde{I}^1)} \Big|_{\text{ref}} (\tilde{I}^1 - (\tilde{I}^1)_o) + \frac{\partial({}^q\tilde{\alpha})}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta) \quad (7.20)$$

As before  $(\tilde{I}^1)_o = 0$ . Hence 7.20 reduces to

$${}^q\tilde{\alpha} = {}^q\tilde{\alpha} \Big|_{\text{ref}} + \frac{\partial({}^q\tilde{\alpha})}{\partial(\tilde{I}^1)} \Big|_{\text{ref}} \tilde{I}^1 + \frac{\partial({}^q\tilde{\alpha})}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta) \quad (7.21)$$

Substituting 7.21 into 7.19

$$\bar{\mathbf{q}}^{(0)} = - \left( {}^q\tilde{\alpha} \Big|_{\text{ref}} + \frac{\partial({}^q\tilde{\alpha})}{\partial(\tilde{I}^1)} \Big|_{\text{ref}} \tilde{I}^1 + \frac{\partial({}^q\tilde{\alpha})}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta) \right) \bar{\mathbf{g}} \quad (7.22)$$

which can be written as

$$\bar{\mathbf{q}}^{(0)} = -{}^q\tilde{\alpha} \Big|_{\text{ref}} \bar{\mathbf{g}} - \frac{\partial({}^q\tilde{\alpha})}{\partial(\tilde{I}^1)} \Big|_{\text{ref}} \tilde{I}^1 \bar{\mathbf{g}} - \frac{\partial({}^q\tilde{\alpha})}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta) \bar{\mathbf{g}} \quad (7.23)$$

Substituting for  $\tilde{I}^1$  yields

$$\bar{\mathbf{q}}^{(0)} = -{}^q\tilde{\alpha} \Big|_{\text{ref}} \bar{\mathbf{g}} - \frac{\partial({}^q\tilde{\alpha})}{\partial(\tilde{I}^1)} \Big|_{\text{ref}} (\bar{\mathbf{g}} \cdot \bar{\mathbf{g}}) \bar{\mathbf{g}} - \frac{\partial({}^q\tilde{\alpha})}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta) \bar{\mathbf{g}} \quad (7.24)$$

Equation 7.24 holds regardless of whether the solid is compressible or incompressible. This is the most general form of the constitutive relations for the heat vector with the assumed form for  $\bar{\mathbf{q}}^{(0)}$  in 7.19.

#### Co-variant basis

Since  $\bar{\mathbf{g}}$  contain Cartesian components, it is straight forward to conclude that  $\bar{\mathbf{q}}^{(0)} = \bar{\mathbf{q}}_{(0)}$ .

### 7.4 Standard Fourier heat conduction law: compressible

Since  $\bar{\mathbf{g}}$  contain Cartesian components, it is straight forward to conclude that  $\bar{\mathbf{q}}^{(0)} = \bar{\mathbf{q}}_{(0)}$ . If we neglect infinitesimals of order two and higher in the components of  $\bar{\mathbf{g}}$  and if we neglect the last term in 7.24, then 7.24 reduces to

$$\bar{\mathbf{q}}^{(0)} = -{}^q\tilde{\alpha} \Big|_{\text{ref}} \bar{\mathbf{g}} \quad (7.25)$$

Let us define

$$k(\bar{\rho}, \bar{\theta}) = {}^q\tilde{\alpha} \Big|_{\text{ref}} \quad (7.26)$$

Then 7.25 becomes

$$\bar{\mathbf{q}}^{(0)} = -k(\bar{\rho}, \bar{\theta}) \bar{\mathbf{g}} = -k(\bar{\rho}, \bar{\theta}) [I] \bar{\mathbf{g}} = -[K(\bar{\rho}, \bar{\theta})] \bar{\mathbf{g}} \quad (7.27)$$

in which  $k(\bar{\rho}, \bar{\theta})$  is thermal conductivity and  $[K(\bar{\rho}, \bar{\theta})]$  is the diagonal thermal conductivity matrix. 7.27 is the standard Fourier heat conduction law.

## 8 Constitutive equation for the heat vector: incompressible

Following section 6, for incompressible medium we have

$$\text{div}(\mathbf{v}) = 0 \quad (8.1)$$

due to continuity equation which implies that

$$\text{tr}([\gamma^{(1)}]) = \text{tr}([\gamma_{(1)}]) = \text{tr}([\gamma^{(0)}]) = \text{tr}([\gamma_{(0)}]) = 0 \quad (8.2)$$

or alternatively, since  $\bar{\rho} = \rho = \text{constant}$ , then

$$\det[J] = 1 \quad (8.3)$$

must hold for incompressible matter. If we consider both, contra-variant and co-variant bases, then we have the following for ordered thermoelastic solids.

$$\bar{\mathbf{q}}^{(0)} = \bar{\mathbf{q}}^{(0)}([\gamma^{(j)}]; j = 1, 2, \dots, n, \bar{\theta}, \bar{\mathbf{g}}) \quad (8.4)$$

$$\bar{\mathbf{q}}_{(0)} = \bar{\mathbf{q}}_{(0)}([\gamma_{(j)}]; j = 1, 2, \dots, n, \bar{\theta}, \bar{\mathbf{g}}) \quad (8.5)$$

The general constitutive theory for heat vectors  $\bar{\mathbf{q}}^{(0)}$  and  $\bar{\mathbf{q}}_{(0)}$  presented in section 7 for ordered thermoelastic solids, i.e., thermoelastic compressible solids of order two and one, can be easily modified for this case by imposing restrictions 8.1 - 8.3 due to incompressibility. Likewise the constitutive equation for heat vector for generalized hypo-thermoelastic compressible solids can also be easily modified using 8.1 - 8.3 due to the fact that 7.24 holds regardless of whether the solid is compressible or incompressible. Details are straight forward and hence are omitted.

### Standard Fourier heat conduction law: incompressible

If we assume that

$$\bar{\mathbf{q}}^{(0)} = \bar{\mathbf{q}}^{(0)}(\bar{\theta}, \bar{\mathbf{g}}) \quad (8.6)$$

$$\text{and } \bar{\mathbf{q}}_{(0)} = \bar{\mathbf{q}}_{(0)}(\bar{\theta}, \bar{\mathbf{g}}) \quad (8.7)$$

then, analogous to the compressible case, we obtain the Fourier heat conduction law. Details are exactly parallel to the compressible case except that in this case  $\rho = \bar{\rho} = \text{constant}$  and hence the coefficient defined by 7.26 in the constitutive equation must be modified accordingly. Thus

$$k(\bar{\theta}) = {}^a \tilde{\alpha} \Big|_{\text{ref}} \quad (8.8)$$

Then 7.25 becomes

$$\bar{\mathbf{q}}^{(0)} = -k(\bar{\theta}) \bar{\mathbf{g}} = -k(\bar{\theta})[I] \bar{\mathbf{g}} = -[K(\bar{\theta})] \bar{\mathbf{g}} \quad (8.9)$$

in which  $k(\bar{\theta})$  is thermal conductivity and  $[K(\bar{\theta})]$  is the diagonal thermal conductivity matrix. 8.9 is the standard Fourier heat conduction law for incompressible matter. Since  $\bar{\mathbf{g}}$  contain Cartesian components, it is straight forward to conclude that  $\bar{\mathbf{q}}^{(0)} = \bar{\mathbf{q}}_{(0)}$ .

## 9 Summary and conclusions

The rate constitutive theory for incompressible as well as compressible ordered thermoelastic solids have been presented in contra-variant and co-variant bases using Eulerian description. When the mathematical models for deforming solids are constructed using Eulerian description, the displacements of the material particles, and hence strain measures, are not readily obtainable. Thus the constitutive theory expressing chosen stress measures as a function of the conjugate strain measure is not possible. Hence, in this situation, one must

consider a relationship between conjugate pairs of stress and strain rates, therefore the need for rate constitutive theory.

Based on the axiom of admissibility, all constitutive equations must satisfy conservation laws to ensure thermodynamic equilibrium of the deforming matter. Since conservation of mass, balance of momenta and energy equation only require existence of the stress field and heat vector, these are independent of the constitution of the matter. Thus the second law of thermodynamics (Clausius-Duhem inequality) must provide the basis for the theory of constitutive equations. The conditions resulting from the Clausius-Duhem inequality show that  $\eta$ , specific entropy is deterministic from the Helmholtz free energy and hence should not be considered as a dependent variable in the constitutive theory; thus, the Cauchy stress tensor, heat vector and the Helmholtz free energy density are the only dependent variables in the constitutive theory for the type of matter considered here. The conditions also provide a mechanism to determine the heat vector as a function of the temperature gradient vector and conductivity, i.e., Fourier heat condition law. However, the conditions do not provide a mechanism to determine constitutive equations for the total Cauchy stress tensor. However, if the total Cauchy stress tensor is decomposed into equilibrium stress and deviatoric stress, then the equilibrium stress is deterministic from the entropy inequality and leads to thermodynamic pressure for compressible matter and mechanical pressure in the case of incompressible matter. These hold regardless of the order of the rate constitutive equations. But the deviatoric Cauchy stress is not deterministic from the entropy inequality, however the entropy inequality does require the dissipation due to the deviatoric Cauchy stress to be positive. Thus the rate constitutive theory for ordered thermoelastic solids reduces to deviatoric Cauchy stress tensor, heat vector and Helmholtz free energy density as dependent variables and their determination using the argument tensors describing the physics of deformation in contra-variant and co-variant bases.

Details of the contra- and co-variant bases, stress and strain measures, convected time derivatives of the stress and strain tensors in contra- and co-variant bases, derivations of entropy inequality and the conditions resulting from it have been presented in reference [1]. It is shown that for compressible ordered thermoelastic solids, in contra-variant basis, the argument tensors of the first convected time derivative of the deviatoric Cauchy stress  $[_d\bar{\sigma}^{(0)}]$ , i.e.,  $[_d\bar{\sigma}^{(1)}]$  and the heat vector  $\bar{\mathbf{q}}^{(0)}$  are  $\bar{\rho}$ ,  $\bar{\theta}$ ,  $\bar{\mathbf{g}}$  and  $[\gamma^{(j)}]$ ;  $j = 1, 2, \dots, n$ , the convected time derivatives of orders  $1, 2, \dots, n$  in the contra-variant basis and for  $\bar{\Phi}$ , the argument tensors are  $\bar{\rho}$  and  $\bar{\theta}$ . In co-variant basis, the argument tensors of the first convected time derivative of the deviatoric Cauchy stress  $[_d\bar{\sigma}_{(0)}]$ , i.e.,  $[_d\bar{\sigma}_{(1)}]$  and the heat vector  $\bar{\mathbf{q}}_{(0)}$  are  $\bar{\rho}$ ,  $\bar{\theta}$ ,  $\bar{\mathbf{g}}$  and  $[\gamma_{(j)}]$ ;  $j = 1, 2, \dots, n$ , the convected time derivatives of orders  $1, 2, \dots, n$  in the co-variant basis and for  $\bar{\Phi}$ , the argument tensors are  $\bar{\rho}$  and  $\bar{\theta}$ . For incompressible ordered thermoelastic solids, density  $\bar{\rho}$  in the current configuration is the same as in the reference configuration and hence it is no longer an argument of the dependent variables in the constitutive theory. Other arguments remain the same as for the compressible case.

The theory of generators and invariants is utilized to derive the general form of the constitutive equations for an  $n^{th}$  order ‘ordered thermoelastic solid’ (both compressible and incompressible) in contra-variant and co-variant bases. In this theory both the first convected time derivative of the deviatoric Cauchy stress and the heat vector are expressed as a linear combination of the combined generators of the argument tensors. The coefficients in this linear combination are functions of the combined invariants of the argument tensors in addition to  $\bar{\rho}$  and  $\bar{\theta}$  (in case of compressible solids) or  $\bar{\theta}$  (in case of incompressible solids). The coefficients in the linear combinations are determined by using their Taylor’s series expansion about the reference configuration and retaining only up to linear terms in the combined invariants and temperature. Explicit details are presented for second order ‘ordered thermoelastic solids’. The general form of the constitutive equations are specialized and detailed derivations are presented for thermoelastic solids of order two and one as well as hypo-thermoelastic solids.

We note that the rate constitutive theory derived here for an ordered thermoelastic solid of order ‘ $n$ ’ express the first convected time derivative of the Cauchy stress tensor as a function of density  $\bar{\rho}$ , temperature  $\bar{\theta}$ , temperature gradient  $\bar{\mathbf{g}}$  and the convected time derivatives of the conjugate strain tensor of up to order ‘ $n$ ’ in a chosen basis, i.e., contra- or -co-variant. The contra-variant basis yields upper convected rate constitutive equations whereas co-variant basis gives lower convected rate constitutive equations. Surana et al. [10] have shown that in the case of finite deformation, only upper convected rate constitutive theory is in conformity with the physics of deformation. Based on the rate constitutive theory presented in this chapter for ordered thermoelastic solids we make the following specific remarks.

1. Definitions of  $[_d\bar{\sigma}^{(1)}]$  and  $[_d\bar{\sigma}_{(1)}]$  differ when the deformation is finite. Furthermore, the definition of

$[\bar{\sigma}^{(1)}]$  is different for compressible and incompressible matter. Same is the case for  $[\bar{\sigma}_{(1)}]$ . In the case of compressible matter  $[\bar{\sigma}^{(1)}]$  is the Truesdell rate.

2. For ordered thermoelastic solids of order greater than or equal to two, the argument tensors  $[\gamma^{(1)}]$  and  $[\gamma_{(1)}]$  are the same but the argument tensors  $[\gamma^{(j)}]; j = 2, 3, \dots$  and  $[\gamma_{(j)}]; j = 2, 3, \dots$  differ.
3. Based on remarks 1. and 2., the rate constitutive equations in contra-variant and co-variant bases are not the same if we deviate from the infinitesimal deformation assumption.
4. Based on the theory of generators and invariants, the constitutive equation for the heat vector for an ordered thermoelastic solid is much more complex (even for thermoelastic solids of order one due to the dependence of the heat vector on the combined generators of  $[\gamma^{(1)}]$ ,  $\bar{\mathbf{g}}$  or  $[\gamma_{(1)}]$ ,  $\bar{\mathbf{g}}$ ) compared to Fourier heat conduction law which requires that the heat vector not be dependent on  $[\gamma^{(1)}]$  or  $[\gamma_{(1)}]$ . The constitutive equation for the heat vector based on the combined generators of  $[\gamma^{(1)}]$ ,  $\bar{\mathbf{g}}$  or  $[\gamma_{(1)}]$ ,  $\bar{\mathbf{g}}$  is perhaps more realistic for finite deformation of solids as it accounts for velocity gradients.
5. When the first order rate constitutive equations ( $n = 1$ ) are simplified to obtain constitutive equations for what is commonly known as hypo-elastic material, the restriction of infinitesimal deformation must be observed. To be more precise, in this case, second and higher order terms in the components of the first convected time derivatives of the strain tensor are assumed negligible. Thus, use of such constitutive relations [30, 31] for finite deformation is not justified.
6. We point out that Jaumann rate constitutive equations are probably most widely used for deforming solid matter in Eulerian description [30, 31]. Surana et al. [1, 10] have shown that Jaumann rate constitutive equations are average of contra- and co-variant descriptions when the velocity field is the same in both bases. This is only true if the deformation is not finite. Nonetheless, these have been used widely for finite deformation [30, 31].
7. It is significant to note that based on Surana et al. [10], when the deformation is finite, only the constitutive equations derived using contra-variant basis remain valid. As the magnitude of the deformation increases, the constitutive equations in co-variant basis and others (such as Jaumann rate equations) become progressively more spurious.
8. The condition of positive dissipation resulting from the entropy inequality is satisfied by all rate constitutive equations presented here provided we observe certain restrictions on the coefficients.
9. Since the constitutive theory in this chapter is based on combined generators and invariants of the argument tensors of the dependent variable, strictly speaking it lacks thermodynamic basis (as these are not derived using entropy inequality). However, the theory does have continuum mechanics foundation and it does satisfy the conditions resulting from entropy inequality.

The work presented here provides a completely general and unified theory for ordered thermoelastic solids from which specialized behaviors such second order theory, first order theory or hypo-elastic constitutive equations can be derived. It is demonstrated that the distinction between contra- and co-variant bases is critical for ordered thermoelastic solids of any order including order one.

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## Chapter 4

# Rate Constitutive Theory for Ordered Thermoviscoelastic Fluids - Polymers

In this chapter we present development of rate constitutive theory for compressible as well as incompressible polymeric fluids. The polymeric fluids in this chapter are considered as ordered thermoviscoelastic fluids in which the stress rate of a desired order, i.e., the convected time derivative of a desired order ' $m$ ' of the chosen deviatoric Cauchy stress tensor, and the heat vector are functions of density, temperature, temperature gradient, convected time derivatives of the chosen strain tensor up to any desired order ' $n$ ' and the convected time derivative of up to orders ' $m - 1$ ' of the chosen deviatoric Cauchy stress tensor. The development of the constitutive theory is presented in both contra-variant as well as co-variant bases. The polymeric fluids described by this constitutive theory will be referred to as ordered thermoviscoelastic fluids due to the fact that the constitutive equations are dependent on the orders ' $m$ ' and ' $n$ ' of the convected time derivatives of the deviatoric Cauchy stress and strain tensors. The highest orders of the convected time derivative of the deviatoric Cauchy stress and strain tensors define the orders of the polymeric fluid.

The admissibility requirement necessitates that the constitutive theory must satisfy conservation laws: conservation of mass, balance of momenta, conservation of energy and the second law of thermodynamics (Clausius-Duhem inequality). Since the first three conservation laws are independent of the constitution of the matter, the entropy inequality must be explored for the development of the constitutive theory. If we decompose the total Cauchy stress tensor into equilibrium stress and deviatoric Cauchy stress, the entropy inequality indeed provides a mechanism for establishing the equilibrium stress as thermodynamic pressure for compressible fluids and mechanical pressure for the incompressible case, with the additional requirement that the dissipation due to the deviatoric Cauchy stress be positive. However, the entropy inequality provides no mechanism for the determination of the constitutive theory for the deviatoric Cauchy stress.

It is shown that in the development of the constitutive theory one must consider a coordinate system in the current configuration in which the deformed material lines can be identified. Thus the co-variant and contra-variant convected coordinate systems are natural choices for the development of the constitutive equations. Furthermore, the mathematical models for fluids require Eulerian description with velocities as dependent variables. This precludes the use of displacement gradients, i.e., strain measures, in the development of the constitutive theory for such matter. It is shown that compatible conjugate pairs of convected time derivatives of the stress and strain measures in co- and contra-variant bases in conjunction with the theory of generators and invariants provide a general mathematical framework for the development of constitutive theory for ordered thermoviscoelastic fluids. This framework has a foundation based on the basic principles and axioms of continuum mechanics and satisfies the condition of positive dissipation, a requirement resulting from the entropy inequality. We present a general theory of constitutive equations for ordered thermoviscoelastic fluids which is then specialized to obtain commonly used constitutive equations for Maxwell, Giesekus and Oldroyd-B constitutive models in contra- and co-variant bases.

The research work presented in this chapter is being submitted for journal publication [1].

# 1 Introduction

The thermoviscoelastic fluids or polymeric fluids are both viscous and elastic. Such fluids consist of a solvent and a polymer. The solvent is a very dilute solution that may be primarily viewed as Newtonian fluid. Its composition is due to short chain molecules. The polymer on the other hand consists of long chain molecules. It has its own viscosity in addition to elasticity. In thermoviscoelastic fluids, the elastic effects are primarily due to the polymer. When a polymeric fluid is subjected to a disturbance, the motion of the polymer molecules is complex (Brownian motion [2, 3]). The polymeric fluids can be classified in two broad categories: dilute polymeric fluids and dense polymeric fluids or polymer melts. Compressibility in polymeric fluids is only important at very high pressures. Generally, polymeric fluids are treated as incompressible, hence it is appropriate to say polymeric liquids. Dilute polymeric fluids are primarily much like Newtonian fluids but with some elastic effects, i.e., the behavior is dominated by viscous effects. In such fluids the solvent viscosity is dominant, i.e., much higher than the polymer viscosity. Polymer melts on the other hand are dense polymeric fluids whose behavior is dominated by elastic effects. In such fluids the polymer viscosity is much higher than the solvent viscosity. Polymeric liquids are of significant industrial importance.

The first attempt to obtain constitutive equations for viscoelastic liquids appears to have been due to Maxwell [4]. Later these were generalized to remove the small displacement assumption [5]. Maxwell constitutive model is a linear viscoelastic model. Using Maxwell model as a basis, the Jeffreys model is obtained by adding time derivative of the symmetric part of the velocity gradient tensor [5, 6]. Generalization of the Maxwell model is obtained by superposition of a series of Maxwell models [5]. It is commonly accepted [5] that linear viscoelastic models have many limitations: (1) They can not describe shear rate dependent viscosity (2) They can not describe normal stress behavior (3) They fail to describe small-strain phenomena if it is accompanied by large displacements due to rigid rotations. This leads to the development of ‘Quasi-linear differential models’ using convected time derivatives. The Oldroyd-B [7] model falls into this category. Deficiencies of these models in describing realistic physical flow phenomena in polymer melts lead to the development of non-linear differential constitutive models for polymeric fluids. Giesekus model [8] and PTT model [9, 10] fall into this category. Many other constitutive models have been proposed for polymeric fluids (see reference [5]). The fundamental driving principles behind these models have been anisotropic drag due to Brownian motion of polymer molecules and their networks and the kinetic theory [11].

First, we remark that polymeric fluids at a macro scale are viewed as isotropic homogeneous continuous media. Thus, in our view, the constitutive equations for such fluids must be derivable using principles and axioms of continuum mechanics constitutive theory. In fact, Maxwell constitutive model has been derived in reference [12, 13] using the theory of generators and invariants. To our knowledge, derivations of Oldroyd-B, Giesekus and other constitutive models based on principles of continuum mechanics are not reported in the published works. It is instructive to examine the derivations of these models based on continuum mechanics principles and as a subset of ordered polymeric fluids as it may suggest new possibilities for improved constitutive models.

## Scope of work

This chapter presents a general theory of rate constitutive equations for ordered thermoviscoelastic fluids, both compressible and incompressible in co- and contra-variant bases based on the principles and axioms of continuum mechanics. The Maxwell, Giesekus and Oldroyd-B constitutive models used currently are derived as special cases of the general rate theory.

At the onset of the development of the constitutive theory, the choice of stress tensor and heat vector as dependent variables is rather obvious. We begin all developments with the second law of thermodynamics (entropy inequality), an essential conservation law for the development of the constitutive theory. Entropy inequality requires that we decompose the total Cauchy stress tensor in equilibrium stress tensor and deviatoric stress tensor. The constitutive equations for the equilibrium stress in case of compressible as well as incompressible polymeric liquids are established using entropy inequality [14]. The constitutive equation for the deviatoric Cauchy stress can not be determined using entropy inequality as it provides no mechanism for doing so except that it requires the dissipation due to the deviatoric Cauchy stress be positive. For deriving the constitutive theory for the deviatoric Cauchy stress, we utilize the theory of generators and invariants [12, 13, 15–25]. In a chosen basis, the convected time derivative of order ‘ $m$ ’ of the deviatoric Cauchy stress tensor is expressed

in terms of the density  $\bar{\rho}$ , temperature  $\bar{\theta}$ , temperature gradient  $\bar{\mathbf{g}}$ , convected time derivatives of the conjugate strain tensor (Almansi or Green) of up to order ' $n$ ' and the convected time derivatives of the deviatoric Cauchy stress tensor of up to order ' $m - 1$ ' as argument tensors. The combined generators (that are symmetric tensors of rank two) and invariants of the argument tensors provide the mechanism for establishing the rate constitutive equations for the deviatoric Cauchy stress tensor in the chosen basis.

In case of the heat vector we also consider  $\bar{\rho}$ ,  $\bar{\theta}$ ,  $\bar{\mathbf{g}}$ , convected time derivatives of the strain tensor of up to order  $n$  and convected time derivatives of the deviatoric Cauchy stress tensor of up to order  $m - 1$  as argument tensors. The combined generators (that are tensors of rank one) and invariants of the argument tensors provide the foundation for establishing the constitutive equations for the heat vector in the chosen basis.

The general derivation of the rate constitutive theory for the deviatoric Cauchy stress and the heat vector are specialized to derive upper convected (contra-variant basis) and lower convected (co-variant basis) rate constitutive equations for Maxwell, Giesekus and Oldroyd-B fluids.

## 2 Preliminary material

In chapter 2 and a recent paper [14] the authors have presented details of notations, contra- and co-variant bases, measures of strains for finite deformation, measures of stress, convected time derivatives of Almansi and Green's strains in co- and contra-variant bases, convected time derivatives of the deviatoric Cauchy stress tensor for compressible and incompressible media in co- and contra-variant basis, derivation of Clausius-Duhem inequality and the conditions resulting from it as well as their consequences in the development of constitutive equations. A summary of these derivations and details is also given in chapter 3 and another recent paper by the authors [26]. Hence this material is not repeated or reproduced in this chapter.

## 3 Considerations in the development of the rate constitutive theory

In reference [14], authors have presented a detailed account of entropy inequality, conditions resulting from it, determination of dependent variables in the constitutive theory and their argument tensors for the development of the rate constitutive equations for ordered thermofluids. A summary of these has also been presented by the authors in reference [26]. The summary in reference [26] is crucial in understanding the clear choices that one must make and paths that one must take in the development of the rate constitutive theory for fluids under consideration. Since these were considered for ordered thermoelastic solids, some modifications are necessary in their use for ordered thermoviscoelastic fluids considered in the work presented here.

The development of the constitutive theory must be based on axioms or principles of continuum mechanics [12, 13, 27]. Thus, the constitutive equations must satisfy conservation laws. Since conservation of mass, balance of momenta, and the first law of thermodynamics only require existence of the stress field and heat vector without considering the constitution of the matter, these are applicable to all deforming matters within the assumption of thermodynamic equilibrium. Additionally, all deforming matter must also satisfy the second law of thermodynamics in order to ensure thermodynamic equilibrium during the evolution. Thus the use of the entropy inequality is a possibility in the development of the constitutive theory for all deforming matter. From the entropy inequality we can deduce the following: (i) conditions that ensure that entropy inequality is not violated (ii) the dependent variables in the constitutive theory. Using the conditions resulting from the entropy inequality and the determination of the dependent variables, we explore the possibility of developing the constitutive theory.

The choice of Lagrangian or Eulerian description is immaterial for the entropy inequality, due to the fact that the dependent variables are transformable from one description to the other. Thus we consider entropy inequality in Lagrangian description [14].

$$\rho \left( \frac{\partial \Phi}{\partial t} + \eta \frac{\partial \theta}{\partial t} \right) + \frac{|J| \underline{q}_i \underline{g}_i}{\theta} - \sigma_{ki}^* \dot{J}_{ik} \leq 0 \quad (3.1)$$

in which  $\Phi$  and  $\eta$  are Helmholtz free energy density and entropy density. From the balance of momenta and the first law of thermodynamics we note that the stress tensor and the heat vector are obviously related to the constitution of the matter and hence must be considered as dependent variables in the constitutive theory. In

3.1 we note the appearance of  $\Phi$  and  $\eta$  as additional dependent variables. Thus, based on the four conservation laws, the stress tensor, heat vector, Helmholtz free energy density and the entropy density must be considered as dependent variables in the development of the constitutive theory. We note that 3.1 contains material derivative of the Helmholtz free energy density. Thus it is necessary to determine the arguments of  $\Phi$  and likewise the arguments of the stress tensor and heat vector in the entropy inequality. Let  $\boldsymbol{\sigma}$ ,  $\mathbf{q}$ ,  $\Phi$  and  $\eta$  and  $\bar{\boldsymbol{\sigma}}$ ,  $\bar{\mathbf{q}}$ ,  $\bar{\Phi}$  and  $\bar{\eta}$  be the dependent variables in the constitutive theory in Lagrangian and Eulerian descriptions (more specific definitions and choices will be considered in the later sections).

Based on the principles of equipresence [12, 13, 27] we consider all possible measures of deformation as arguments of the four dependent variables. The Jacobian of deformation  $[J]$  is fundamental in the kinematics of deformation of any matter and hence must be an argument in each of the four dependent variables. Since we are considering fluids,  $[\dot{J}]$  (time or material derivative of  $[J]$ ) must be an argument as well [14]. Temperature is obviously an argument. In addition to these three, we also consider  $\mathbf{g}$ , the temperature gradient, as an argument. Thus we have

$$\begin{aligned}\boldsymbol{\sigma} &= \boldsymbol{\sigma}([J], [\dot{J}], \theta, \mathbf{g}) \\ \mathbf{q} &= \mathbf{q}([J], [\dot{J}], \theta, \mathbf{g}) \\ \Phi &= \Phi([J], [\dot{J}], \theta, \mathbf{g}) \\ \eta &= \eta([J], [\dot{J}], \theta, \mathbf{g})\end{aligned}\tag{3.2}$$

If in 3.2 the independent variables are  $(x_i, t)$ , then these are in Lagrangian or material descriptions in which case  $\boldsymbol{\sigma}$  may represent first Piola-Kirchhoff stress, or second Piola-Kirchhoff stress (Cartesian components of the contra-variant Cauchy stress tensor), or Cartesian components of the co-variant Cauchy stress tensor. On the other hand, if the independent variables are  $(\bar{x}_i, t)$ , then these are in Eulerian or spatial description in which case  $\boldsymbol{\sigma}$  may represent contra- or co-variant Cauchy stress tensor. Now, since we have arguments of  $\Phi$ , we can consider a more detailed form of entropy inequality 3.1 by using

$$\frac{\partial \Phi}{\partial t} = \frac{\partial \Phi}{\partial J_{ik}} \dot{J}_{ik} + \frac{\partial \Phi}{\partial \dot{J}_{ik}} \ddot{J}_{ik} + \frac{\partial \Phi}{\partial \theta} \dot{\theta} + \frac{\partial \Phi}{\partial g_i} \dot{g}_i\tag{3.3}$$

Substituting 3.3 in 3.1

$$\rho \left( \frac{\partial \Phi}{\partial J_{ik}} \dot{J}_{ik} + \frac{\partial \Phi}{\partial \dot{J}_{ik}} \ddot{J}_{ik} + \frac{\partial \Phi}{\partial \theta} \dot{\theta} + \frac{\partial \Phi}{\partial g_i} \dot{g}_i + \eta \frac{\partial \theta}{\partial t} \right) + \frac{|J| \underline{q}_i \underline{g}_i}{\theta} - \sigma_{ki}^* \dot{J}_{ik} \leq 0\tag{3.4}$$

$$\text{or } \rho \frac{\partial \Phi}{\partial \dot{J}_{ik}} \ddot{J}_{ik} + \left( \rho \frac{\partial \Phi}{\partial J_{ik}} - \sigma_{ki}^* \right) \dot{J}_{ik} + \rho \left( \frac{\partial \Phi}{\partial \theta} + \eta \right) \dot{\theta} + \frac{|J| \underline{q}_i \underline{g}_i}{\theta} + \frac{\partial \Phi}{\partial g_i} \dot{g}_i \leq 0\tag{3.5}$$

In order for 3.5 to hold for arbitrary (but admissible)  $[\ddot{J}]$ ,  $\dot{\theta}$  and  $\dot{\mathbf{g}}$ , the following must hold:

$$\rho \frac{\partial \Phi}{\partial \dot{J}_{ik}} = 0\tag{3.6}$$

$$\frac{\partial \Phi}{\partial g_i} = 0\tag{3.7}$$

$$\frac{\partial \Phi}{\partial \theta} + \eta = 0\tag{3.8}$$

$$\text{and } \left( \rho \frac{\partial \Phi}{\partial J_{ik}} - \sigma_{ki}^* \right) \dot{J}_{ik} + \frac{|J| \underline{q}_i \underline{g}_i}{\theta} \leq 0\tag{3.9}$$

Equations 3.6 - 3.9 are fundamental relations from the second law of thermodynamics (or entropy inequality).

**Remarks:**

- (1) 3.6 implies that  $\Phi$  is not a function of  $[\dot{J}]$ .

- (2) 3.7 implies that  $\Phi$  is not a function of  $\mathbf{g}$  either.
- (3) Based on 3.8,  $\eta$  is not a dependent variable in the constitutive theory as  $\eta = -\frac{\partial \Phi}{\partial \theta}$ , hence  $\eta$  is deterministic from  $\Phi$ .
- (4) The inequality in the last equation 3.9 is essential in the form it is stated. For example

$$\rho \frac{\partial \Phi}{\partial J_{ik}} - \sigma_{ki}^* = 0 \quad \text{and} \quad \frac{|J| \underline{q_i} \underline{g_i}}{\theta} \leq 0$$

are inappropriate due to the fact that these imply that  $[\sigma^*]$  is not a function of  $[\dot{J}]$  which is contrary to 3.2. Thus 3.9 in its stated form is unable to provide us further details regarding the constitutive equations for  $[\sigma^*]$  and  $\mathbf{q}$ .

In order to alleviate the situation discussed in remark (4), we consider decomposition of  $[\sigma^*]$  into equilibrium stress  $[{}_e\sigma^*]$  and deviatoric stress  $[{}_d\sigma^*]$ , i.e.

$$[\sigma^*] = [{}_e\sigma^*] + [{}_d\sigma^*] \quad (3.10)$$

At this stage we can only conclude the following:

$$[{}_e\sigma^*] = [{}_e\sigma^*([J], [0], \theta, \mathbf{g})] \quad (3.11)$$

$$[{}_d\sigma^*] = [{}_d\sigma^*([J], [\dot{J}], \theta, \mathbf{g})] \quad (3.12)$$

That is,  $[{}_e\sigma^*]$  is not a function of  $[\dot{J}]$  and  $[{}_d\sigma^*]$  vanishes when  $[\dot{J}]$  and  $\mathbf{g}$  are zero. Substituting from 3.10 into 3.9 gives

$$\left( \rho \frac{\partial \Phi}{\partial J_{ik}} - {}_e\sigma_{ki}^* - {}_d\sigma_{ki}^* \right) \dot{J}_{ik} + \frac{|J| \underline{q_i} \underline{g_i}}{\theta} \leq 0 \quad (3.13)$$

Since  $\Phi$  is not a function of  $[\dot{J}]$  and neither is  ${}_e\sigma_{ik}^*$  (3.11), then  ${}_e\sigma_{ik}^*$  must be derivable from

$${}_e\sigma_{ki}^* = \rho \frac{\partial \Phi}{\partial J_{ik}} \quad (3.14)$$

Using 3.14, the inequality 3.13 reduces to

$$-{}_d\sigma_{ki}^* \dot{J}_{ik} + \frac{|J| \underline{q_i} \underline{g_i}}{\theta} \leq 0 \quad (3.15)$$

If we assume (as done routinely to derive Fourier heat conduction law [12–14, 27])

$$\frac{|J| \underline{q_i} \underline{g_i}}{\theta} \leq 0 \quad (3.16)$$

Then 3.15 is satisfied if the following holds:

$${}_d\sigma_{ki}^* \dot{J}_{ik} > 0 \quad (3.17)$$

Equation 3.17 requires that conversion of mechanical energy must be positive. Thus 3.10 can be written as

$$\sigma_{ij}^* = \rho \frac{\partial \Phi}{\partial J_{ki}} + {}_d\sigma_{ij}^*([J], [\dot{J}], \theta, \mathbf{g}) \quad (3.18)$$

$$\text{and} \quad \Phi = \Phi([J], \theta) \quad (3.19)$$

$$\mathbf{q} = \mathbf{q}([J], [\dot{J}], \theta, \mathbf{g}) \quad (3.20)$$

Derivation of Fourier heat conduction law for  $\mathbf{q}$  is straight forward based on 3.16 [12–14, 27]. A more general derivation is presented in a subsequent section.

## Further consideration on the argument tensors

We note that in Eulerian description, transformation of its reference frame by a unimodular (orthogonal) matrix cannot be detected by its subsequent thermomechanical deformation. Thus if  $x$ -frame changes to  $x'$ -frame via

$$\{x'\} = [R]\{x\} \quad (3.21)$$

$$\therefore [J'] = [J][R]^t \quad (3.22)$$

Then, based on the principle of frame invariance

$$\Phi([J], \theta) = \Phi([J'], \theta) = \Phi([J][R]^t, \theta) \quad (3.23)$$

must hold and likewise, the principle of frame invariance must also hold for the stress and heat vector. But this is only possible if  $\Phi$ , the stress tensor and heat vector depend upon  $|J|$  and not  $[J]$  due to the fact that,

$$\det[J'] = \det([J][R]^t) = \det[J] \det[R]^t = \det[J] \quad (3.24)$$

is frame invariant. Furthermore, we note that

$$\begin{aligned} [\dot{J}] &= [L][J] \quad ; \quad [D] = \frac{1}{2}([L] + [L]^t) \quad ; \quad [W] = \frac{1}{2}([L] - [L]^t) \\ \therefore [L] &= [D] + [W] \quad \text{and} \quad [\dot{J}] = ([D] + [W])[J] \end{aligned} \quad (3.25)$$

Thus dependence of the stress tensor and heat vector on  $[\dot{J}]$  can be replaced by the dependence on  $|J|$ ,  $[D]$  and  $[W]$ . But  $[W]$  is pure rotation and hence dependence on  $[W]$  can be eliminated. Thus the stress tensor and heat vector must have dependence on  $|J|$ ,  $[D]$ ,  $\theta$  and  $\mathbf{g}$ . We note that

- (1) From conservation of mass

$$\rho = |J|\bar{\rho} \quad \text{or} \quad |J| = \frac{\rho}{\bar{\rho}} \quad (3.26)$$

in which  $\rho$  is constant (density in the reference configuration). Thus  $|J|$  can be replaced with  $1/\bar{\rho}$  or simply  $\bar{\rho}$ .

- (2) Since for fluids, Eulerian description is necessary, we have two obvious choices: contra-variant basis or co-variant basis and hence contra-variant Cauchy stress  $[\bar{\sigma}^{(0)}]$  or co-variant Cauchy stress  $[\bar{\sigma}_{(0)}]$  tensors are obvious choices in the constitutive theory.
- (3) Recalling the derivations of the convected time derivatives of Green's strain in co-variant basis, we note that  $[D]$  is the convected time derivative of order one of the Green's strain in co-variant basis, i.e.

$$[D] = [\gamma_{(1)}] \quad (3.27)$$

which is also the convected time derivative of order zero (by definition). Thus

$$[D] = [\gamma_{(0)}] = [\gamma_{(1)}] \quad (3.28)$$

By definition,  $[\gamma_{(0)}]$  and  $[\gamma_{(1)}]$  are fundamental kinematic tensors of order zero and one in co-variant basis derived based on Green's strain tensor, a co-variant measure of finite strain.

- (4) Likewise if we consider the convected time derivatives of the Almansi strain in contra-variant basis, we note that  $[D]$  is also the convected time derivative of order one of the Almansi strain in contra-variant basis, i.e.

$$[D] = [\gamma^{(1)}] \quad (3.29)$$

which is also the convected time derivative of order zero (by definition). Thus

$$[D] = [\gamma^{(0)}] = [\gamma^{(1)}] \quad (3.30)$$

By definition,  $[\gamma^{(0)}]$  and  $[\gamma^{(1)}]$  are fundamental kinematic tensors of order zero and one in contra-variant basis derived using Almansi strain tensor, a contra-variant measure of finite strain.

- (5) We have seen that convected time derivatives of order higher than one of the Green's strain tensor and Almansi strain tensor can be derived in co-variant and contra-variant bases which are fundamental kinematic tensors of various orders in the respective bases. Thus

$$[\gamma^{(j)}] \quad ; \quad j = 1, 2, \dots, n \quad (3.31)$$

$$\text{and} \quad [\gamma_{(j)}] \quad ; \quad j = 1, 2, \dots, n \quad (3.32)$$

are fundamental kinematic tensors in contra- and co-variant bases. Hence, to generalize the development of the constitutive theory, these must replace  $[D]$  in the argument tensors for the dependent variables in the constitutive theory.

- (6) From the Maxwell model, Giesekus model, Oldroyd-B model etc. we note that these models contain convected time derivatives of orders one and zero. Thus these must be derivable by considering the first convected time derivative of the deviatoric Cauchy stress as a dependent variable in the constitutive theory in which the convected time derivative of order zero of the deviatoric Cauchy stress is an argument tensor (see later sections). In the work presented here we generalize this concept and consider the convected time derivative of order ' $m$ ' of the chosen deviatoric Cauchy stress tensor (co- or contra-variant basis) as a dependent variable in the constitutive theory with convected time derivatives of up to order ' $m - 1$ ' of the same deviatoric stress tensor as its arguments in addition to the other argument tensors.

With considerations (1) to (6), we now have finalized the dependent variables and their argument tensors in the rate constitutive theory.

In Eulerian description, co-variant and contra-variant bases are obviously two clear choices for the development of the constitutive theory. In the following we consider these two bases and the choice of dependent variables and their argument tensors for the compressible and incompressible case.

### 3.1 Final choice of the argument tensors: compressible

#### Contra-variant basis:

The conjugate pairs of the convected time derivatives of the deviatoric Cauchy stress tensor and fundamental kinematic tensors in the contra-variant basis are

$$\begin{aligned} [{}_d\bar{\sigma}^{(k)}] & \quad ; \quad k = 0, 1, \dots, m \\ [\gamma^{(j)}] & \quad ; \quad j = 1, 2, \dots, n \end{aligned} \quad (3.33)$$

and we have the following for the dependent variables in the constitutive theory.

$$\bar{\Phi} = \bar{\Phi}(\bar{\rho}(\bar{\mathbf{x}}, t), \bar{\theta}(\bar{\mathbf{x}}, t)) \quad (3.34)$$

$$\begin{aligned} [{}_d\bar{\sigma}^{(m)}] &= [{}_d\bar{\sigma}^{(m)}(\bar{\rho}(\bar{\mathbf{x}}, t), [{}_d\sigma^{(k)}(\bar{\mathbf{x}}, t)] ; k = 0, 1, \dots, m-1, \\ &\quad [\gamma^{(j)}(\bar{\mathbf{x}}, t)] ; j = 1, 2, \dots, n, \bar{\theta}(\bar{\mathbf{x}}, t), \bar{\mathbf{g}}(\bar{\mathbf{x}}, t))] \end{aligned} \quad (3.35)$$

$$[\bar{\sigma}^{(0)}] = [{}_e\bar{\sigma}^{(0)}] + [{}_d\bar{\sigma}^{(0)}] \quad (3.36)$$

$$\begin{aligned} \bar{\mathbf{q}}^{(0)} &= \bar{\mathbf{q}}^{(0)}(\bar{\rho}(\bar{\mathbf{x}}, t), [{}_d\sigma^{(k)}(\bar{\mathbf{x}}, t)] ; k = 0, 1, \dots, m-1, \\ &\quad [\gamma^{(j)}(\bar{\mathbf{x}}, t)] ; j = 1, 2, \dots, n, \bar{\theta}(\bar{\mathbf{x}}, t), \bar{\mathbf{g}}(\bar{\mathbf{x}}, t)) \end{aligned} \quad (3.37)$$

$$\text{and} \quad [{}_e\sigma^*]^t = \rho(\mathbf{x}, t) \frac{\partial \Phi(\rho(\mathbf{x}, t), \theta(\mathbf{x}, t))}{\partial [J(\mathbf{x}, t)]} \quad (3.38)$$

#### Co-variant basis:

The conjugate pairs of the convected time derivatives of the deviatoric Cauchy stress tensor and fundamental kinematic tensors in the co-variant basis are

$$\begin{aligned} [{}_d\bar{\sigma}_{(k)}] & \quad ; \quad k = 0, 1, \dots, m \\ [\gamma_{(j)}] & \quad ; \quad j = 1, 2, \dots, n \end{aligned} \quad (3.39)$$

and we have the following for the dependent variables in the constitutive theory.

$$\bar{\Phi} = \bar{\Phi}(\bar{\rho}(\bar{\mathbf{x}}, t), \bar{\theta}(\bar{\mathbf{x}}, t)) \quad (3.40)$$

$$[{}_d\bar{\sigma}_{(m)}] = [{}_d\bar{\sigma}_{(m)}(\bar{\rho}(\bar{\mathbf{x}}, t), [{}_d\sigma_{(k)}(\bar{\mathbf{x}}, t)]; k = 0, 1, \dots, m-1, \\ [\gamma_{(j)}(\bar{\mathbf{x}}, t)]; j = 1, 2, \dots, n, \bar{\theta}(\bar{\mathbf{x}}, t), \bar{\mathbf{g}}(\bar{\mathbf{x}}, t)] \quad (3.41)$$

$$[\bar{\sigma}_{(0)}] = [{}_e\bar{\sigma}_{(0)}] + [{}_d\bar{\sigma}_{(0)}] \quad (3.42)$$

$$\bar{\mathbf{q}}_{(0)} = \bar{\mathbf{q}}_{(0)}(\bar{\rho}(\bar{\mathbf{x}}, t), [{}_d\sigma_{(k)}(\bar{\mathbf{x}}, t)]; k = 0, 1, \dots, m-1, \\ [\gamma_{(j)}(\bar{\mathbf{x}}, t)]; j = 1, 2, \dots, n, \bar{\theta}(\bar{\mathbf{x}}, t), \bar{\mathbf{g}}(\bar{\mathbf{x}}, t)) \quad (3.43)$$

$$\text{and } [{}_e\sigma^*]^t = \rho(\mathbf{x}, t) \frac{\partial \Phi(\rho(\mathbf{x}, t), \theta(\mathbf{x}, t))}{\partial [J(\mathbf{x}, t)]} \quad (3.44)$$

### 3.2 Final choice of the argument tensors: incompressible

For incompressible matter  $\bar{\rho} = \rho = \text{constant}$ . Thus we have the following for contra-variant and co-variant bases.

#### Contra-variant basis:

The conjugate pairs of the convected time derivatives of the deviatoric Cauchy stress tensor and fundamental kinematic tensors in the contra-variant basis are

$$[{}_d\bar{\sigma}^{(k)}] \quad ; \quad k = 0, 1, \dots, m \\ [\gamma^{(j)}] \quad ; \quad j = 1, 2, \dots, n \quad (3.45)$$

The derivation of  $[{}_e\sigma^*]$  for incompressible matter presented in reference [14] holds here precisely and hence is omitted. Thus we have the following for the dependent variables in the constitutive theory.

$$\bar{\Phi} = \bar{\Phi}(\bar{\rho}(\bar{\theta}(\bar{\mathbf{x}}, t))) \quad (3.46)$$

$$[{}_d\bar{\sigma}^{(m)}] = [{}_d\bar{\sigma}^{(m)}([{}_d\sigma^{(k)}(\bar{\mathbf{x}}, t)]; k = 0, 1, \dots, m-1, \\ [\gamma^{(j)}(\bar{\mathbf{x}}, t)]; j = 1, 2, \dots, n, \bar{\theta}(\bar{\mathbf{x}}, t), \bar{\mathbf{g}}(\bar{\mathbf{x}}, t))] \quad (3.47)$$

$$[\bar{\sigma}^{(0)}] = [{}_e\bar{\sigma}^{(0)}] + [{}_d\bar{\sigma}^{(0)}] \quad (3.48)$$

$$\bar{\mathbf{q}}^{(0)} = \bar{\mathbf{q}}^{(0)}([{}_d\sigma^{(k)}(\bar{\mathbf{x}}, t)]; k = 0, 1, \dots, m-1, \\ [\gamma^{(j)}(\bar{\mathbf{x}}, t)]; j = 1, 2, \dots, n, \bar{\theta}(\bar{\mathbf{x}}, t), \bar{\mathbf{g}}(\bar{\mathbf{x}}, t)) \quad (3.49)$$

$$\text{and } [{}_e\sigma^*] = \rho(\mathbf{x}, t)[J(\mathbf{x}, t)]^{-1} \quad (3.50)$$

#### Co-variant basis:

The conjugate pairs of the convected time derivatives of the deviatoric Cauchy stress tensor and fundamental kinematic tensors in the co-variant basis are

$$[{}_d\bar{\sigma}_{(k)}] \quad ; \quad k = 0, 1, \dots, m \\ [\gamma_{(j)}] \quad ; \quad j = 1, 2, \dots, n \quad (3.51)$$

As in the case of contra-variant basis, the derivation of  $[{}_e\sigma^*]$  for incompressible matter presented in reference [14] holds here precisely. Thus we have the following for the dependent variables in the constitutive theory.

$$\bar{\Phi} = \bar{\Phi}(\bar{\rho}(\bar{\theta}(\bar{\mathbf{x}}, t))) \quad (3.52)$$

$$[{}_d\bar{\sigma}_{(m)}] = [{}_d\bar{\sigma}_{(m)}(\bar{\rho}(\bar{\theta}(\bar{\mathbf{x}}, t)); k = 0, 1, \dots, m-1, [\gamma_{(j)}(\bar{\mathbf{x}}, t)]; j = 1, 2, \dots, n, \bar{\theta}(\bar{\mathbf{x}}, t), \bar{\mathbf{g}}(\bar{\mathbf{x}}, t))] \quad (3.53)$$

$$[\bar{\sigma}_{(0)}] = [{}_e\bar{\sigma}_{(0)}] + [{}_d\bar{\sigma}_{(0)}] \quad (3.54)$$

$$\bar{\mathbf{q}}_{(0)} = \bar{\mathbf{q}}_{(0)}(\bar{\rho}(\bar{\theta}(\bar{\mathbf{x}}, t)); k = 0, 1, \dots, m-1, [\gamma_{(j)}(\bar{\mathbf{x}}, t)]; j = 1, 2, \dots, n, \bar{\theta}(\bar{\mathbf{x}}, t), \bar{\mathbf{g}}(\bar{\mathbf{x}}, t)) \quad (3.55)$$

$$\text{and } [{}_e\sigma^*] = \rho(\mathbf{x}, t)[J(\mathbf{x}, t)]^{-1} \quad (3.56)$$

In the following sections we consider specific details of rate constitutive theory in the two bases for compressible and incompressible cases.

## 4 Development of the rate constitutive theory for the Cauchy stress tensor

### 4.1 Equilibrium stress $[{}_e\bar{\sigma}^{(0)}]$ or $[{}_e\bar{\sigma}_{(0)}]$

The development of the constitutive equations for the equilibrium stress requires the use of 3.14 and transformation of  $[\sigma^*]$  to  $[{}_e\bar{\sigma}^{(0)}]$  or  $[{}_e\bar{\sigma}_{(0)}]$ . The derivation presented in reference [14] holds here precisely and hence is not repeated. We only present the final forms.

**Compressible thermoviscoelastic fluids:**

$$[{}_e\bar{\sigma}^{(0)}] = [{}_e\bar{\sigma}_{(0)}] = p(\bar{\rho}, \bar{\theta})[I] \quad (4.1)$$

i.e., equilibrium stress is independent of the choice of basis.  $p(\bar{\rho}, \bar{\theta})$  is thermodynamic pressure defined by the equation of state.

**Incompressible thermoviscoelastic fluids:**

$$[{}_e\bar{\sigma}^{(0)}] = [{}_e\bar{\sigma}_{(0)}] = p(\bar{\theta})[I] \quad (4.2)$$

in which  $p(\bar{\theta})$  is mechanical pressure.  $p(\bar{\theta})$  is not deterministic from the deformation field.

In equations 4.1 and 4.2 we can replace  $p(\bar{\rho}, \bar{\theta})$  and  $p(\bar{\theta})$  by  $-p(\bar{\rho}, \bar{\theta})$  and  $-p(\bar{\theta})$  if we assume compressive pressure to be positive.

### 4.2 Deviatoric Cauchy stress $[{}_d\bar{\sigma}^{(0)}]$ or $[{}_d\bar{\sigma}_{(0)}]$

In this section we consider constitutive theory for the deviatoric Cauchy stress in contra- and co-variant bases.

**Compressible thermoviscoelastic fluids:**

Based on 3.10 and 4.1 we have the following for compressible polymers

$$[\bar{\sigma}^{(0)}] = p(\bar{\rho}, \bar{\theta})[I] + [{}_d\bar{\sigma}^{(0)}] \quad (4.3)$$

$$[\bar{\sigma}_{(0)}] = p(\bar{\rho}, \bar{\theta})[I] + [{}_d\bar{\sigma}_{(0)}] \quad (4.4)$$

in which

$$\begin{aligned} [{}_d\bar{\sigma}^{(m)}] &= [{}_d\bar{\sigma}^{(m)}(\bar{\rho}, [{}_d\sigma^{(k)}]; k = 0, 1, \dots, m-1, [\gamma^{(j)}]; j = 1, 2, \dots, n, \bar{\theta}, \bar{\mathbf{g}})] \\ [{}_d\bar{\sigma}_{(m)}] &= [{}_d\bar{\sigma}_{(m)}(\bar{\rho}, [{}_d\sigma_{(k)}]; k = 0, 1, \dots, m-1, [\gamma_{(j)}]; j = 1, 2, \dots, n, \bar{\theta}, \bar{\mathbf{g}})] \end{aligned} \quad (4.5)$$

### Incompressible thermoviscoelastic fluids:

Based on 3.10 and 4.2 we have the following for incompressible polymers

$$[\bar{\sigma}^{(0)}] = p(\bar{\theta})[I] + [{}_d\bar{\sigma}^{(0)}] \quad (4.6)$$

$$[\bar{\sigma}_{(0)}] = p(\bar{\theta})[I] + [{}_d\bar{\sigma}_{(0)}] \quad (4.7)$$

in which

$$\begin{aligned} [{}_d\bar{\sigma}^{(m)}] &= [{}_d\bar{\sigma}^{(m)}([{}_d\sigma^{(k)}]; k = 0, 1, \dots, m-1, [\gamma^{(j)}]; j = 1, 2, \dots, n, \bar{\theta}, \bar{\mathbf{g}})] \\ [{}_d\bar{\sigma}_{(m)}] &= [{}_d\bar{\sigma}_{(m)}([{}_d\sigma_{(k)}]; k = 0, 1, \dots, m-1, [\gamma_{(j)}]; j = 1, 2, \dots, n, \bar{\theta}, \bar{\mathbf{g}})] \end{aligned} \quad (4.8)$$

First, we make some remarks [14] that are helpful in understanding the approach used for deriving the constitutive theory for the deviatoric Cauchy stress tensor in contra- and co-variant bases.

- (1)  $[{}_d\bar{\sigma}^{(k)}]$  and  $[{}_d\bar{\sigma}_{(k)}]; k = 0, 1, \dots, m$  are symmetric tensors of rank two.  $[\gamma^{(j)}]$  and  $[\gamma_{(j)}]; j = 1, 2, \dots, n$  are symmetric fundamental kinematic tensors of rank two;  $\bar{\rho}, \bar{\theta}$  are tensors of rank zero and  $\bar{\mathbf{g}}$  is a tensor of rank one.
- (2)  $[{}_d\bar{\sigma}^{(k)}], [{}_d\bar{\sigma}_{(k)}]; k = 0, 1, \dots, m, [\gamma^{(j)}], [\gamma_{(j)}]; j = 1, 2, \dots, n$  and  $\bar{\mathbf{g}}$  have their own invariants but also there exist combined invariants between them.
- (3) In the case of homogeneous and isotropic compressible fluids, the equilibrium stress (thermodynamic pressure) is completely deterministic from the entropy inequality once we define Helmholtz free energy density in terms of the invariants of the chosen strain measure. In the case of homogeneous and isotropic incompressible fluids, the equilibrium stress (mechanical pressure) is also derived from the entropy inequality in conjunction with incompressibility constraint, however, the equilibrium stress is not a function of the Helmholtz free energy density and it is not deterministic from the deformation field. Furthermore, the second law of thermodynamics only restricts the dissipative energy (entropy production) due to the deviatoric stress to be positive but provides no mechanism for determining the constitutive theory for the deviatoric Cauchy stress.
- (4) The theory of generators and invariants [15–25] provides a continuum mechanics foundation to derive the constitutive theory for the deviatoric stress. This theory utilizes a linear combination of the combined generators (of the same rank as the deviatoric stress) of the argument tensors of rank one and two to describe the deviatoric stress tensor field. The coefficients in the linear combinations are functions of combined invariants of the argument tensors, temperature  $\bar{\theta}$  and density  $\bar{\rho}$  which are then determined by using Taylor series expansion of the coefficients about the reference configuration. Thus, in principle, this approach is quite straight forward.
- (5) Based on (4), the key element in the theory of generators and invariants is the determination of the minimal basis using the combined generators of the argument tensors and of course, determination of the combined invariants. For example  $[T([S])]$ , where  $[T]$  and  $[S]$  are symmetric tensors of rank two, which obey the invariance

$$[T([R][S][R]^t)] = [R][T([S])][R]^t \quad (4.9)$$

has the form

$$[T] = \alpha_0[I] + \alpha_1[S] + \alpha_2[S]^2 \quad (4.10)$$

where  $\alpha_0, \alpha_1$  and  $\alpha_2$  are functions of the invariants of  $[S]$ , i.e.,  $\text{tr}([S])$ ,  $\text{tr}([S]^2)$  and  $\text{tr}([S]^3)$  called principal invariants, or the invariants  $I_s, \mathbb{I}_s$  and  $\mathbb{III}_s$  from the characteristic equation of  $[S]$ . The tensors  $[I], [S], [S]^2$  are called generators of the tensor  $[T]$  and form the minimal basis. If the arguments of  $[T]$  consist of more than one tensor (could be of different rank), then a linear combination like 4.10 would contain all combined generators (of the same rank as  $[T]$ ) of the argument tensors and likewise the coefficients in the linear combination would be functions of the combined invariants. For details on the combined generators and invariants for various combinations of the argument tensors see references [15–25].

- (6) Based on the remarks presented above, we now have a basis for deriving the constitutive theory for the deviatoric stress as well as the heat vector. In the following we consider contra-variant as well as co-variant bases, keeping in mind that the heat vector is a tensor of rank one and hence the combined generators of its argument tensors must also be of rank one.
- (7) We reiterate that the following form the basis of the rate constitutive equations for the deviatoric Cauchy stress tensor for compressible as well as incompressible ordered thermoviscoelastic fluids using the theory of generators and invariants:

### Compressible polymeric fluids:

For the compressible case, we consider the following for the  $m^{th}$  convected time derivative of the deviatoric Cauchy stress tensor in contra- and co-variant basis.

$$[{}_d\bar{\sigma}^{(m)}] = [{}_d\bar{\sigma}^{(m)}(\bar{\rho}, [\bar{\sigma}^{(k)}]; k = 0, 1, \dots, m-1, [\gamma^{(j)}]; j = 1, 2, \dots, n, \bar{\theta}, \bar{\mathbf{g}})] \quad (4.11)$$

$$[{}_d\bar{\sigma}_{(m)}] = [{}_d\bar{\sigma}_{(m)}(\bar{\rho}, [\bar{\sigma}_{(k)}]; k = 0, 1, \dots, m-1, [\gamma_{(j)}]; j = 1, 2, \dots, n, \bar{\theta}, \bar{\mathbf{g}})] \quad (4.12)$$

### Incompressible polymeric fluids:

For the incompressible case the density is constant, hence we consider the following for the  $m^{th}$  convected time derivative of the deviatoric Cauchy stress tensor in contra- and co-variant basis.

$$[{}_d\bar{\sigma}^{(m)}] = [{}_d\bar{\sigma}^{(m)}([\bar{\sigma}^{(k)}]; k = 0, 1, \dots, m-1, [\gamma^{(j)}]; j = 1, 2, \dots, n, \bar{\theta}, \bar{\mathbf{g}})] \quad (4.13)$$

$$[{}_d\bar{\sigma}_{(m)}] = [{}_d\bar{\sigma}_{(m)}([\bar{\sigma}_{(k)}]; k = 0, 1, \dots, m-1, [\gamma_{(j)}]; j = 1, 2, \dots, n, \bar{\theta}, \bar{\mathbf{g}})] \quad (4.14)$$

4.11 - 4.14 must form the basis for deriving the constitutive theory for the deviatoric Cauchy stress in contra- and co-variant bases.

In the following we present details of the constitutive theory based on 4.11 - 4.14 for compressible and incompressible polymeric fluids in contra- and co-variant bases using theory of generators and invariants.

## 5 Development of the rate constitutive theory for the deviatoric Cauchy stress tensor

We consider a general theory of the rate constitutive equations in contra- and co-variant bases in which the convected time derivative of order ' $m$ ' of the deviatoric Cauchy stress tensor contains: (i) convected time derivatives of up to order ' $m-1$ ' of the deviatoric Cauchy stress tensor (ii) convected time derivatives of the strain tensor of up to order ' $n$ ' (iii) density  $\bar{\rho}$ , temperature  $\bar{\theta}$  and temperature gradient  $\bar{\mathbf{g}}$  as argument tensors in the chosen basis. These fluids are considered ordered fluids of orders  $(m-1, n)$ . Details are presented in the following.

### 5.1 Contra-variant basis

First we consider compressible thermoviscoelastic polymeric fluids, in which we have

$$[{}_d\bar{\sigma}^{(m)}] = [{}_d\bar{\sigma}^{(m)}(\bar{\rho}, [{}_d\bar{\sigma}^{(k)}]; k = 0, 1, \dots, m-1, [\gamma^{(j)}]; j = 1, 2, \dots, n, \bar{\theta}, \bar{\mathbf{g}})] \quad (5.1)$$

We note that  $[{}_d\bar{\sigma}^{(k)}]; k = 0, 1, \dots, m-1$  and  $[\gamma^{(j)}]; j = 1, 2, \dots, n$  are symmetric tensors of rank two and  $\bar{\mathbf{g}}$  is a tensor of rank one. Let  $[\sigma G^i]; i = 1, 2, \dots, N$  be the combined generators (symmetric tensors of rank two, due to the fact that  $[{}_d\bar{\sigma}^{(m)}]$  is a symmetric tensor of rank two) of the tensors  $[{}_d\bar{\sigma}^{(k)}]; k = 0, 1, \dots, m-1$  and  $[\gamma^{(j)}]; j = 1, 2, \dots, n$  and  $\bar{\mathbf{g}}$ . Let  ${}^{q\sigma}I^j; j = 1, 2, \dots, M$  be the combined invariants of the same

tensors [12, 13, 15–25]. Now we can express  $[d\bar{\sigma}^{(m)}]$  as a linear combination of  $[I]$  and the generators  $[\sigma G^i]$ ;  $i = 1, 2, \dots, N$ .

$$[d\bar{\sigma}^{(m)}] = \sigma_{\alpha}^0 [I] + \sum_{i=1}^N \sigma_{\alpha}^i [\sigma G^i] \quad (5.2)$$

The coefficients  $\sigma_{\alpha}^i$ ;  $i = 0, 1, \dots, N$  are functions of the combined invariants  ${}^{q\sigma}I_j$ ;  $j = 1, 2, \dots, M$ , density  $\bar{\rho}$  and temperature  $\bar{\theta}$ . The coefficients  $\sigma_{\alpha}^i$ ;  $i = 0, 1, \dots, N$  are determined by using Taylor series expansion for each  $\sigma_{\alpha}^i$  about the reference configuration and only retaining up to linear terms in the combined invariants  ${}^{q\sigma}I_j$  and temperature  $\bar{\theta}$ .

$$\sigma_{\alpha}^i = \sigma_{\alpha}^i \Big|_{\text{ref}} + \sum_{j=1}^M \frac{\partial(\sigma_{\alpha}^i)}{\partial({}^{q\sigma}I_j)} \Big|_{\text{ref}} ({}^{q\sigma}I_j - ({}^{q\sigma}I_j)_0) + \frac{\partial(\sigma_{\alpha}^i)}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 0, 1, \dots, N \quad (5.3)$$

in which the quantities with the subscript zero are their values in the reference configuration. We note that  $({}^{q\sigma}I_j)_0$ ;  $j = 1, 2, \dots, M$  are all zero in the reference configuration and  $\bar{\mathbf{g}}|_0 = 0$  if we assume that the fluid in the reference configuration only has uniform temperature field. Hence, we obtain the following from 5.3.

$$\sigma_{\alpha}^i = \sigma_{\alpha}^i \Big|_{\text{ref}} + \sum_{j=1}^M \frac{\partial(\sigma_{\alpha}^i)}{\partial({}^{q\sigma}I_j)} \Big|_{\text{ref}} {}^{q\sigma}I_j + \frac{\partial(\sigma_{\alpha}^i)}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 0, 1, \dots, N \quad (5.4)$$

Substituting from 5.4 into 5.2 gives the most general form of the constitutive relations for  $[d\bar{\sigma}^{(m)}]$  for thermo-viscoelastic compressible polymeric fluids of orders  $(m, n)$  in contra-variant basis. The coefficients in the final expression are functions of density  $\bar{\rho}$  and temperature  $\bar{\theta}$ .

If the fluid is considered incompressible, then density  $\bar{\rho}$  is no longer an argument of the dependent variables in the constitutive theory and we have

$$[d\bar{\sigma}^{(m)}] = [d\bar{\sigma}^{(m)}]({}^{q\sigma}I_j; j = 1, 2, \dots, n, \bar{\theta}, \bar{\mathbf{g}}) \quad (5.5)$$

The rest of the details follow the compressible case except for the dependence of the coefficients on density  $\bar{\rho}$ . In the final expression for the convected time derivative of order ‘ $m$ ’ of the deviatoric Cauchy stress tensor, the coefficients are only functions of temperature  $\bar{\theta}$ .

## 5.2 Co-variant basis

In this case for compressible thermoviscoelastic polymeric fluids we have

$$[d\bar{\sigma}_{(m)}] = [d\bar{\sigma}_{(m)}](\bar{\rho}, [d\bar{\sigma}_{(k)}]; k = 0, 1, \dots, m-1, [\gamma_{(j)}]; j = 1, 2, \dots, n, \bar{\theta}, \bar{\mathbf{g}}) \quad (5.6)$$

Here also (as in the case of contra-variant basis)  $[\bar{\sigma}_{(k)}]$ ;  $k = 0, 1, \dots, m-1$  and  $[\gamma_{(j)}]$ ;  $j = 1, 2, \dots, n$  are symmetric tensors of rank two and  $\bar{\mathbf{g}}$  is a tensor of rank one. Let  $[\sigma G_i]$ ;  $i = 1, 2, \dots, N$  be the combined generators (symmetric tensors of rank two) of the tensors  $[d\bar{\sigma}_{(k)}]$ ;  $k = 0, 1, \dots, m-1$  and  $[\gamma_{(j)}]$ ;  $j = 1, 2, \dots, n$  and  $\bar{\mathbf{g}}$ . Let  ${}^{q\sigma}I_j$ ;  $j = 1, 2, \dots, M$  be the combined invariants of the same tensors [12, 13, 15–25]. Now we can express  $[d\bar{\sigma}_{(m)}]$  as a linear combination of  $[I]$  and the generators  $[\sigma G_i]$ ;  $i = 1, 2, \dots, N$ .

$$[d\bar{\sigma}_{(m)}] = \sigma_{\alpha 0} [I] + \sum_{i=1}^N \sigma_{\alpha i} [\sigma G_i] \quad (5.7)$$

The coefficients  $\sigma_{\alpha i}$ ;  $i = 0, 1, \dots, N$  are functions of the combined invariants  ${}^{q\sigma}I_j$ ;  $j = 0, 1, \dots, M$ , density  $\bar{\rho}$  and temperature  $\bar{\theta}$ . The coefficients  $\sigma_{\alpha i}$ ;  $i = 0, 1, \dots, N$  are determined by using Taylor series expansion for each  $\sigma_{\alpha i}$  about the reference configuration and only retaining up to linear terms in the combined invariants  ${}^{q\sigma}I_j$  and temperature  $\bar{\theta}$ .

$$\sigma_{\alpha i} = \sigma_{\alpha i} \Big|_{\text{ref}} + \sum_{j=1}^M \frac{\partial(\sigma_{\alpha i})}{\partial({}^{q\sigma}I_j)} \Big|_{\text{ref}} ({}^{q\sigma}I_j - ({}^{q\sigma}I_j)_0) + \frac{\partial(\sigma_{\alpha i})}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 0, 1, \dots, N \quad (5.8)$$

As in the case of contra-variant basis, here also,  $({}^{q\sigma}I_j)_0 = 0$  ;  $j = 1, 2, \dots, M$  due to the fact that  $[d\bar{\sigma}_{(k)}]$  ;  $k = 0, 1, \dots, m-1$  and  $[\gamma_{(j)}]$  ;  $j = 1, 2, \dots, n$  are all zero in the reference configuration and  $\bar{\mathbf{g}} = 0$  if we assume that the fluid in the reference configuration only has uniform temperature field. Hence 5.8 reduces to

$$\sigma_{\alpha_i} = \sigma_{\alpha_i} \Big|_{\text{ref}} + \sum_{j=1}^M \frac{\partial(\sigma_{\alpha_i})}{\partial({}^{q\sigma}I_j)} \Big|_{\text{ref}} {}^{q\sigma}I_j + \frac{\partial(\sigma_{\alpha_i})}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 0, 1, \dots, N \quad (5.9)$$

Substituting from 5.9 into 5.7 gives the most general form of the constitutive relations for  $[d\bar{\sigma}_{(m)}]$  for thermo-viscoelastic compressible polymeric fluids of orders  $(m, n)$  in co-variant basis. The coefficients in the final expressions are functions of density  $\bar{\rho}$  and temperature  $\bar{\theta}$ .

If the fluid is considered incompressible, then  $\bar{\rho} = \rho = \text{constant}$ . Thus density  $\bar{\rho}$  is no longer an argument of the dependent variables in the constitutive theory and we have

$$[d\bar{\sigma}_{(m)}] = [d\bar{\sigma}_{(m)}]([d\bar{\sigma}_{(k)}] ; k = 0, 1, \dots, m-1, [\gamma_{(j)}] ; j = 1, 2, \dots, n, \bar{\theta}, \bar{\mathbf{g}}) \quad (5.10)$$

The rest of the details follow the compressible case except for the dependence of the coefficients on density  $\bar{\rho}$ . In the final expression for the convected time derivative of order ‘ $m$ ’ of the deviatoric Cauchy stress tensor, the coefficients are only functions of temperature  $\bar{\theta}$ .

### 5.3 Special forms of rate constitutive equations for compressible and incompressible thermoviscoelastic polymeric fluids

The general theory presented in sections 5.1 and 5.2 are specialized in the following sections. We consider rate constitutive equations of order one in deviatoric Cauchy stress and strain rates, i.e.,  $m = 1$  and  $n = 1$ . This derivation forms the basis for Maxwell model and Giesekus model. We also consider rate constitutive equations of order one in deviatoric Cauchy stress and of order two in strain rate, i.e.,  $m = 1$  and  $n = 2$ . This derivation forms the basis for Oldroyd-B model. The derivations are presented in contra- as well as co-variant bases. For the sake of simplicity we drop  $\bar{\mathbf{g}}$  from the argument tensors as commonly done for the widely used constitutive models for polymeric fluids. However, inclusion of  $\bar{\mathbf{g}}$  as argument tensor presents no special difficulty except that the number of combined generators and invariants increase.

In the general derivation we consider the fluid to be compressible and specialize the results for the incompressible case when appropriate.

### 5.4 Rate constitutive equations of order one in deviatoric Cauchy stress and strain rates: $m = n = 1$

#### Contra-variant basis:

In the absence of  $\bar{\mathbf{g}}$  as argument tensor but permitting uniform temperature change from reference to current configuration, we have the following for the first convected time derivative of the deviatoric Cauchy stress tensor in contra-variant basis.

$$[d\bar{\sigma}^{(1)}] = [d\bar{\sigma}^{(1)}](\bar{\rho}, [d\bar{\sigma}^{(0)}], [\gamma^{(1)}], \bar{\theta}) \quad (5.11)$$

The development of the constitutive theory in this case requires: (1) combined generators of  $[d\bar{\sigma}^{(0)}]$  and  $[\gamma^{(1)}]$  (both symmetric tensors of rank two) that are also symmetric tensors of rank two due to the fact that  $[d\bar{\sigma}^{(1)}]$  is a symmetric tensor of rank two (2) combined invariants of the tensors  $[d\bar{\sigma}^{(0)}]$  and  $[\gamma^{(1)}]$ . The combined generators and the invariants are listed in tables 4.1 and 4.2.

#### Remarks:

1. We note that the invariants listed in table 4.2 under (2) marked (a) need not be included due to the fact that

$$\text{tr}([d\bar{\sigma}^{(0)}][\gamma^{(1)}] + [\gamma^{(1)}][d\bar{\sigma}^{(0)}]) + \text{tr}([d\bar{\sigma}^{(0)}][\gamma^{(1)}] - [\gamma^{(1)}][d\bar{\sigma}^{(0)}]) = 2 \text{tr}([d\bar{\sigma}^{(0)}][\gamma^{(1)}])$$

which is same as  ${}^{q\sigma}I^7$  (except for the factor 2 which is of no consequence).

Table 4.1: Combined generators for  $[_d\bar{\sigma}^{(1)}]$ : Maxwell model (contra-variant basis)

Arguments	Generators
(1) none	$[I]$
(2) one at a time ( including (1) )	
$[_d\bar{\sigma}^{(0)}]$	$[\sigma_{\sim}^G{}^1] = [_d\bar{\sigma}^{(0)}] \quad ; \quad [\sigma_{\sim}^G{}^2] = [_d\bar{\sigma}^{(0)}]^2$
$[\gamma^{(1)}]$	$[\sigma_{\sim}^G{}^3] = [\gamma^{(1)}] \quad ; \quad [\sigma_{\sim}^G{}^4] = [\gamma^{(1)}]^2$
(3) two at a time ( including (1) and (2) )	
$[_d\bar{\sigma}^{(0)}] \quad , \quad [\gamma^{(1)}]$	$[\sigma_{\sim}^G{}^5] = [_d\bar{\sigma}^{(0)}][\gamma^{(1)}] + [\gamma^{(1)}][_d\bar{\sigma}^{(0)}]$ $[\sigma_{\sim}^G{}^6] = [_d\bar{\sigma}^{(0)}]^2[\gamma^{(1)}] + [\gamma^{(1)}][_d\bar{\sigma}^{(0)}]^2$ $[\sigma_{\sim}^G{}^7] = [_d\bar{\sigma}^{(0)}][\gamma^{(1)}]^2 + [\gamma^{(1)}]^2[_d\bar{\sigma}^{(0)}]$

2. In many published works (a) are also included in the list of invariants in addition to  ${}^{q\sigma}\tilde{I}^7$  which is redundant.

Using the generators in table 4.1 we can express  $[_d\bar{\sigma}^{(1)}]$  as a linear combination of  $[I]$  and the combined generators  $[\sigma_{\sim}^G{}^i] ; i = 1, 2, \dots, 7$  in the contra-variant basis.

$$[_d\bar{\sigma}^{(1)}] = \sigma_{\alpha}^0[I] + \sum_{i=1}^7 \sigma_{\alpha}^i[\sigma_{\sim}^G{}^i] \quad (5.12)$$

The coefficients  $\sigma_{\alpha}^i ; i = 0, 1, \dots, 7$  are functions of the combined invariants  ${}^{q\sigma}\tilde{I}^j ; j = 1, 2, \dots, 10$ , density  $\bar{\rho}$  and temperature  $\bar{\theta}$ . The coefficients  $\sigma_{\alpha}^i ; i = 0, 1, \dots, 7$  are determined by using Taylor series expansion for each  $\sigma_{\alpha}^i$  about the reference configuration and only retaining up to linear terms in the combined invariants  ${}^{q\sigma}\tilde{I}^j$  and temperature  $\bar{\theta}$ .

$$\sigma_{\alpha}^i = \sigma_{\alpha}^i \Big|_{\text{ref}} + \sum_{j=1}^{10} \frac{\partial(\sigma_{\alpha}^i)}{\partial({}^{q\sigma}\tilde{I}^j)} \Big|_{\text{ref}} ({}^{q\sigma}\tilde{I}^j - ({}^{q\sigma}\tilde{I}^j)_0) + \frac{\partial(\sigma_{\alpha}^i)}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 0, 1, \dots, 7 \quad (5.13)$$

in which the quantities with the subscript zero are their values in the reference configuration. We note that  $({}^{q\sigma}\tilde{I}^j)_0 ; j = 1, 2, \dots, 10$  are all zero due to the fact that  $[_d\bar{\sigma}^{(0)}]$  and  $[\gamma^{(1)}]$  are null in the reference configuration (fluid at rest, i.e., no motion). Hence 5.13 can be written as

$$\sigma_{\alpha}^i = \sigma_{\alpha}^i \Big|_{\text{ref}} + \sum_{j=1}^{10} \frac{\partial(\sigma_{\alpha}^i)}{\partial({}^{q\sigma}\tilde{I}^j)} \Big|_{\text{ref}} {}^{q\sigma}\tilde{I}^j + \frac{\partial(\sigma_{\alpha}^i)}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 0, 1, \dots, 7 \quad (5.14)$$

By substituting 5.14 into 5.12 we obtain the most general form of the first order rate (in stress and strain rates)

Table 4.2: Combined invariants for  $[{}_d\bar{\sigma}^{(1)}]$ : Maxwell model (contra-variant basis)

Arguments	Invariants
(1) one at a time	
$[{}_d\bar{\sigma}^{(0)}]$	${}^{q\sigma}\widetilde{I}^1 = \text{tr}([{}_d\bar{\sigma}^{(0)}])$ ; ${}^{q\sigma}\widetilde{I}^2 = \text{tr}([{}_d\bar{\sigma}^{(0)}]^2)$ ${}^{q\sigma}\widetilde{I}^3 = \text{tr}([{}_d\bar{\sigma}^{(0)}]^3)$
$[\gamma^{(1)}]$	${}^{q\sigma}\widetilde{I}^4 = \text{tr}([\gamma^{(1)}])$ ; ${}^{q\sigma}\widetilde{I}^5 = \text{tr}([\gamma^{(1)}]^2)$ ${}^{q\sigma}\widetilde{I}^6 = \text{tr}([\gamma^{(1)}]^3)$
(2) two at a time ( including (1) )	
$[{}_d\bar{\sigma}^{(0)}]$ , $[\gamma^{(1)}]$	${}^{q\sigma}\widetilde{I}^7 = \text{tr}([{}_d\bar{\sigma}^{(0)}][\gamma^{(1)}])$ ; ${}^{q\sigma}\widetilde{I}^8 = \text{tr}([{}_d\bar{\sigma}^{(0)}]^2[\gamma^{(1)}])$ ${}^{q\sigma}\widetilde{I}^9 = \text{tr}([{}_d\bar{\sigma}^{(0)}][\gamma^{(1)}]^2)$ ; ${}^{q\sigma}\widetilde{I}^{10} = \text{tr}([{}_d\bar{\sigma}^{(0)}]^2[\gamma^{(1)}]^2)$ <div style="border: 1px solid black; padding: 5px; display: inline-block;"> <math>(a) \begin{cases} {}^{q\sigma}\widetilde{I} = \text{tr}([{}_d\bar{\sigma}^{(0)}][\gamma^{(1)}] + [\gamma^{(1)}][{}_d\bar{\sigma}^{(0)}]) \\ {}^{q\sigma}\widetilde{I} = \text{tr}([{}_d\bar{\sigma}^{(0)}][\gamma^{(1)}] - [\gamma^{(1)}][{}_d\bar{\sigma}^{(0)}]) \end{cases}</math> </div>

constitutive theory corresponding to  $m = 1$  and  $n = 1$  in contra-variant basis.

$$\begin{aligned}
 [{}_d\bar{\sigma}^{(1)}] = & \left( \sigma_{\alpha^0} \Big|_{\text{ref}} + \sum_{j=1}^{10} \frac{\partial(\sigma_{\alpha^0})}{\partial({}^{q\sigma}\widetilde{I}^j)} \Big|_{\text{ref}} {}^{q\sigma}\widetilde{I}^j + \frac{\partial(\sigma_{\alpha^0})}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \right) [I] \\
 & + \sum_{i=1}^7 \left( \sigma_{\alpha^i} \Big|_{\text{ref}} + \sum_{j=1}^{10} \frac{\partial(\sigma_{\alpha^i})}{\partial({}^{q\sigma}\widetilde{I}^j)} \Big|_{\text{ref}} {}^{q\sigma}\widetilde{I}^j + \frac{\partial(\sigma_{\alpha^i})}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \right) [{}^{\sigma}G^i]
 \end{aligned} \tag{5.15}$$

We note that this expression for  $[{}_d\bar{\sigma}^{(1)}]$  contains all the combined generators and invariants of the argument tensors listed in tables 4.1 and 4.2. Thus it is a non-linear relationship in  $[{}_d\bar{\sigma}^{(0)}]$  and  $[\gamma^{(1)}]$  but it is a first order rate theory ( $m = 1$  and  $n = 1$ ).

#### Co-variant basis:

Following 5.11, in this case we we have the following for the first convected time derivative of the deviatoric Cauchy stress tensor in co-variant basis.

$$[{}_d\bar{\sigma}_{(1)}] = [{}_d\bar{\sigma}_{(1)}(\bar{\rho}, [{}_d\bar{\sigma}_{(0)}], [\gamma_{(1)}], \bar{\theta})] \tag{5.16}$$

Let  $[{}^{\sigma}G_i]$ ;  $i = 1, 2, \dots, 7$  be the combined generators (symmetric tensors of rank two) of the tensors  $[{}_d\bar{\sigma}_{(0)}]$  and  $[\gamma_{(1)}]$ . These can be obtained using the definitions of  $[{}^{\sigma}G^i]$ ;  $i = 1, 2, \dots, 7$  but by replacing  $[{}_d\bar{\sigma}^{(0)}]$  and  $[\gamma^{(1)}]$  with  $[{}_d\bar{\sigma}_{(0)}]$  and  $[\gamma_{(1)}]$ . Likewise the combined invariants  ${}^{q\sigma}\widetilde{I}_j$ ;  $j = 1, 2, \dots, 10$  can be obtained from the definitions of  ${}^{q\sigma}\widetilde{I}^j$ ;  $j = 1, 2, \dots, 10$  by replacing  $[{}_d\bar{\sigma}^{(0)}]$  and  $[\gamma^{(1)}]$  with  $[{}_d\bar{\sigma}_{(0)}]$  and  $[\gamma_{(1)}]$ . Now we can express  $[{}_d\bar{\sigma}_{(1)}]$  as a linear combination of  $[I]$  and the combined generators  $[{}^{\sigma}G_i]$ ;  $i = 1, 2, \dots, 7$  in the co-variant basis.

$$[{}_d\bar{\sigma}_{(1)}] = \sigma_{\alpha_0}[I] + \sum_{i=1}^7 \sigma_{\alpha_i}[{}^{\sigma}G_i] \tag{5.17}$$

The coefficients  $\sigma_{\alpha_i}$  ;  $i = 0, 1, \dots, 7$  are functions of the combined invariants  ${}^{q\sigma}I_j$  ;  $j = 1, 2, \dots, 10$ , density  $\bar{\rho}$  and temperature  $\bar{\theta}$ . The coefficients  $\sigma_{\alpha_i}$  ;  $i = 0, 1, \dots, 7$  are determined by using Taylor series expansion for each  $\sigma_{\alpha_i}$  about the reference configuration and only retaining up to linear terms in the combined invariants  ${}^{q\sigma}I_j$  and temperature  $\bar{\theta}$ .

$$\sigma_{\alpha_i} = \sigma_{\alpha_i} \Big|_{\text{ref}} + \sum_{j=1}^{10} \frac{\partial(\sigma_{\alpha_i})}{\partial({}^{q\sigma}I_j)} \Big|_{\text{ref}} ({}^{q\sigma}I_j - ({}^{q\sigma}I_j)_0) + \frac{\partial(\sigma_{\alpha_i})}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 0, 1, \dots, 7 \quad (5.18)$$

in which the quantities with the subscript zero are their values in the reference configuration. Since  $({}^{q\sigma}I_j)_0$  ;  $j = 1, 2, \dots, 16$  are zero (for the same reasons as in the contra-variant case) then 5.18 reduces to

$$\sigma_{\alpha_i} = \sigma_{\alpha_i} \Big|_{\text{ref}} + \sum_{j=1}^{10} \frac{\partial(\sigma_{\alpha_i})}{\partial({}^{q\sigma}I_j)} \Big|_{\text{ref}} {}^{q\sigma}I_j + \frac{\partial(\sigma_{\alpha_i})}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 0, 1, \dots, 7 \quad (5.19)$$

By substituting from 5.19 into 5.17 we obtain the most general form of the first order (in stress and strain rates) rate constitutive theory corresponding to  $m = 1$  and  $n = 1$  in co-variant basis.

$$\begin{aligned} [{}_d\bar{\sigma}_{(1)}] = & \left( \sigma_{\alpha_0} \Big|_{\text{ref}} + \sum_{j=1}^{10} \frac{\partial(\sigma_{\alpha_0})}{\partial({}^{q\sigma}I_j)} \Big|_{\text{ref}} {}^{q\sigma}I_j + \frac{\partial(\sigma_{\alpha_0})}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \right) [I] \\ & + \sum_{i=1}^7 \left( \sigma_{\alpha_i} \Big|_{\text{ref}} + \sum_{j=1}^{10} \frac{\partial(\sigma_{\alpha_i})}{\partial({}^{q\sigma}I_j)} \Big|_{\text{ref}} {}^{q\sigma}I_j + \frac{\partial(\sigma_{\alpha_i})}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \right) [{}^\sigma G_i] \end{aligned} \quad (5.20)$$

We note that this expression for  $[{}_d\bar{\sigma}_{(1)}]$  contains all the combined generators and invariants of the argument tensors. Thus it is a non-linear relationship in  $[{}_d\bar{\sigma}_{(0)}]$  and  $[\gamma_{(1)}]$  but it is a first order theory ( $m = 1$  and  $n = 1$ ).

#### Remarks:

1. Based on the general forms 5.15 and 5.20 in contra- and co-variant bases we can derive Maxwell and Giesekus constitutive models in both bases. Details are presented in the following sections.
2. The constitutive equations 5.15 and 5.20 are non-linear partial differential equations in  $[{}_d\bar{\sigma}^{(0)}]$ ,  $[\gamma^{(1)}]$  and  $[{}_d\bar{\sigma}_{(0)}]$ ,  $[\gamma_{(1)}]$ . The constants or the coefficients in 5.15 and 5.20 must be determined experimentally.

#### Maxwell constitutive model

The Maxwell constitutive model is a linear viscoelastic model for dilute polymeric fluids that are generally considered incompressible. Thus, in this constitutive model,  $[{}_d\bar{\sigma}^{(1)}]$  and  $[{}_d\bar{\sigma}_{(1)}]$  must exhibit linear dependence on the generators  $[{}_d\bar{\sigma}^{(0)}]$  or  $[{}_d\bar{\sigma}_{(0)}]$  and  $[\gamma^{(1)}]$  or  $[\gamma_{(1)}]$  depending upon the choice of basis. Furthermore, the coefficients in the linear combination of the generators can only depend upon the first invariants of  $[{}_d\bar{\sigma}^{(0)}]$  or  $[{}_d\bar{\sigma}_{(0)}]$  and  $[\gamma^{(1)}]$  or  $[\gamma_{(1)}]$ . We consider details in the following.

#### Contra-variant basis:

In this case we consider

$$[{}_d\bar{\sigma}^{(1)}] = \sigma_{\alpha^0} [I] + \sigma_{\alpha^1} [{}_d\bar{\sigma}^{(0)}] + \sigma_{\alpha^2} [\gamma^{(1)}] \quad (5.21)$$

The coefficients  $\sigma_{\alpha^i}$  ;  $i = 0, 1, 2$  are not the same as used before but we use the same notation to maintain consistency.  $\sigma_{\alpha^i}$  ;  $i = 0, 1, 2$  are functions of  $i_{_d\bar{\sigma}^{(0)}} = \text{tr}([{}_d\bar{\sigma}^{(0)}])$  and  $i_{\gamma^{(1)}} = \text{tr}([\gamma^{(1)}])$ , the first principal invariants of the tensors  $[{}_d\bar{\sigma}^{(0)}]$  and  $[\gamma^{(1)}]$ , density  $\bar{\rho}$  and temperature  $\bar{\theta}$ . Using Taylor series expansion of each  $\sigma_{\alpha^i}$  about the reference configuration and retaining only up to first order terms in the invariants and temperature we obtain

$$\begin{aligned} \sigma_{\alpha^i} = & \sigma_{\alpha^i} \Big|_{\text{ref}} + \frac{\partial(\sigma_{\alpha^i})}{\partial(i_{_d\bar{\sigma}^{(0)}})} \Big|_{\text{ref}} (i_{_d\bar{\sigma}^{(0)}} - (i_{_d\bar{\sigma}^{(0)}})_0) + \frac{\partial(\sigma_{\alpha^i})}{\partial(i_{\gamma^{(1)}})} \Big|_{\text{ref}} (i_{\gamma^{(1)}} - (i_{\gamma^{(1)}})_0) \\ & + \frac{\partial(\sigma_{\alpha^i})}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 0, 1, 2 \end{aligned} \quad (5.22)$$

The quantities with subscript zero are their values in the reference configuration. Let  $\tilde{\theta} = \bar{\theta} - \theta_0$ . Since  $(i_{d\bar{\sigma}^{(0)}})_0 = (i_{\gamma^{(1)}})_0 = 0$  due to the fact that  $[d\bar{\sigma}^{(0)}]$  and  $[\gamma^{(1)}]$  are null tensors in the reference configuration, 5.22 reduces to

$$\sigma_{\alpha}^i = \sigma_{\alpha}^i \Big|_{\text{ref}} + \frac{\partial(\sigma_{\alpha}^i)}{\partial(i_{d\bar{\sigma}^{(0)}})} \Big|_{\text{ref}} \text{tr}([d\bar{\sigma}^{(0)}]) + \frac{\partial(\sigma_{\alpha}^i)}{\partial(i_{\gamma^{(1)}})} \Big|_{\text{ref}} \text{tr}([\gamma^{(1)}]) + \frac{\partial(\sigma_{\alpha}^i)}{\partial\bar{\theta}} \Big|_{\text{ref}} \tilde{\theta} \quad ; \quad i = 0, 1, 2 \quad (5.23)$$

Substituting from 5.23 into 5.21 gives

$$\begin{aligned} [d\bar{\sigma}^{(1)}] = & \left( \sigma_{\alpha}^0 \Big|_{\text{ref}} + \frac{\partial(\sigma_{\alpha}^0)}{\partial(i_{d\bar{\sigma}^{(0)}})} \Big|_{\text{ref}} \text{tr}([d\bar{\sigma}^{(0)}]) + \frac{\partial(\sigma_{\alpha}^0)}{\partial(i_{\gamma^{(1)}})} \Big|_{\text{ref}} \text{tr}([\gamma^{(1)}]) + \frac{\partial(\sigma_{\alpha}^0)}{\partial\bar{\theta}} \Big|_{\text{ref}} \tilde{\theta} \right) [I] \\ & + \left( \sigma_{\alpha}^1 \Big|_{\text{ref}} + \frac{\partial(\sigma_{\alpha}^1)}{\partial(i_{d\bar{\sigma}^{(0)}})} \Big|_{\text{ref}} \text{tr}([d\bar{\sigma}^{(0)}]) + \frac{\partial(\sigma_{\alpha}^1)}{\partial(i_{\gamma^{(1)}})} \Big|_{\text{ref}} \text{tr}([\gamma^{(1)}]) + \frac{\partial(\sigma_{\alpha}^1)}{\partial\bar{\theta}} \Big|_{\text{ref}} \tilde{\theta} \right) [d\bar{\sigma}^{(0)}] \\ & + \left( \sigma_{\alpha}^2 \Big|_{\text{ref}} + \frac{\partial(\sigma_{\alpha}^2)}{\partial(i_{d\bar{\sigma}^{(0)}})} \Big|_{\text{ref}} \text{tr}([d\bar{\sigma}^{(0)}]) + \frac{\partial(\sigma_{\alpha}^2)}{\partial(i_{\gamma^{(1)}})} \Big|_{\text{ref}} \text{tr}([\gamma^{(1)}]) + \frac{\partial(\sigma_{\alpha}^2)}{\partial\bar{\theta}} \Big|_{\text{ref}} \tilde{\theta} \right) [\gamma^{(1)}] \end{aligned} \quad (5.24)$$

Since the Maxwell model is a linear viscoelastic model, we neglect all terms in 5.24 that contain squares and higher powers of the components of the tensors  $[d\bar{\sigma}^{(0)}]$ ,  $[\gamma^{(1)}]$  and temperature  $\bar{\theta}$  as well as those containing the products of their components. Thus the terms containing  $\text{tr}([d\bar{\sigma}^{(0)}])[d\bar{\sigma}^{(0)}]$ ,  $\text{tr}([\gamma^{(1)}])[d\bar{\sigma}^{(0)}]$ ,  $\tilde{\theta}[d\bar{\sigma}^{(0)}]$ ,  $\text{tr}([d\bar{\sigma}^{(0)}])[\gamma^{(1)}]$ ,  $\text{tr}([\gamma^{(1)}])[\gamma^{(1)}]$  and  $\tilde{\theta}[\gamma^{(1)}]$  in 5.24 are neglected. With these assumptions, 5.24 reduces to the following:

$$\begin{aligned} [d\bar{\sigma}^{(1)}] = & \left( \sigma_{\alpha}^0 \Big|_{\text{ref}} + \frac{\partial(\sigma_{\alpha}^0)}{\partial(i_{d\bar{\sigma}^{(0)}})} \Big|_{\text{ref}} \text{tr}([d\bar{\sigma}^{(0)}]) + \frac{\partial(\sigma_{\alpha}^0)}{\partial(i_{\gamma^{(1)}})} \Big|_{\text{ref}} \text{tr}([\gamma^{(1)}]) + \frac{\partial(\sigma_{\alpha}^0)}{\partial\bar{\theta}} \Big|_{\text{ref}} \tilde{\theta} \right) [I] \\ & + \left( \sigma_{\alpha}^1 \Big|_{\text{ref}} \right) [d\bar{\sigma}^{(0)}] + \left( \sigma_{\alpha}^2 \Big|_{\text{ref}} \right) [\gamma^{(1)}] \end{aligned} \quad (5.25)$$

For simplicity, let us introduce the following new notations

$$\begin{aligned} \bar{\sigma}^0 = \sigma_{\alpha}^0 \Big|_{\text{ref}} \quad ; \quad A_1(\bar{\rho}, \bar{\theta}) = \frac{\partial(\sigma_{\alpha}^0)}{\partial(i_{d\bar{\sigma}^{(0)}})} \Big|_{\text{ref}} \quad ; \quad A_2(\bar{\rho}, \bar{\theta}) = \frac{\partial(\sigma_{\alpha}^0)}{\partial(i_{\gamma^{(1)}})} \Big|_{\text{ref}} \\ A_3(\bar{\rho}, \bar{\theta}) = \sigma_{\alpha}^1 \Big|_{\text{ref}} \quad ; \quad A_4(\bar{\rho}, \bar{\theta}) = \sigma_{\alpha}^2 \Big|_{\text{ref}} \quad ; \quad A_5(\bar{\rho}, \bar{\theta}) = -\frac{\partial(\sigma_{\alpha}^0)}{\partial\bar{\theta}} \Big|_{\text{ref}} \end{aligned} \quad (5.26)$$

Thus 5.25 can be written as

$$[d\bar{\sigma}^{(1)}] = \bar{\sigma}^0 [I] + A_1 \text{tr}([d\bar{\sigma}^{(0)}]) [I] + A_2 \text{tr}([\gamma^{(1)}]) [I] + A_3 [d\bar{\sigma}^{(0)}] + A_4 [\gamma^{(1)}] - A_5 \tilde{\theta} [I] \quad (5.27)$$

This expression is the most general form of linear rate constitutive equation for polymeric fluids (compressible) in contra-variant basis based on the rate constitutive theory of order one in stress and strain rates, i.e.,  $m = 1$  and  $n = 1$ .

To derive Maxwell rate constitutive equation we begin with 5.27 and impose further restrictions on the coefficients. Let us assume  $\bar{\sigma}^0 = 0$  (initial configuration is stress free),  $A_1 = 0$  and  $A_5 = 0$  (no uniform temperature change between reference and current configuration). Then 5.27 reduces to

$$[d\bar{\sigma}^{(1)}] = A_2 \text{tr}([\gamma^{(1)}]) [I] + A_3 [d\bar{\sigma}^{(0)}] + A_4 [\gamma^{(1)}] \quad (5.28)$$

We rearrange terms in 5.28

$$[d\bar{\sigma}^{(0)}] - \frac{1}{A_3} [d\bar{\sigma}^{(1)}] = -\frac{A_4}{A_3} [\gamma^{(1)}] - \frac{A_2}{A_3} \text{tr}([\gamma^{(1)}]) [I] \quad (5.29)$$

and define the following new coefficients

$$\lambda_1 = -\frac{1}{A_3} \quad ; \quad 2\eta_0(\bar{\theta}) = -\frac{A_4}{A_3} \quad ; \quad \kappa_0(\bar{\theta}) = -\frac{A_2}{A_3} \quad (5.30)$$

Thus, with these new definitions, 5.29 can be written as

$$[{}_d\bar{\sigma}^{(0)}] + \lambda_1[{}_d\bar{\sigma}^{(1)}] = 2\eta_0(\bar{\theta})[\gamma^{(1)}] + \kappa_0(\bar{\theta}) \text{tr}([\gamma^{(1)}])[I] \quad (5.31)$$

in which (see reference [14])

$$[{}_d\bar{\sigma}^{(1)}] = \frac{D}{Dt}[{}_d\bar{\sigma}^{(0)}] - [{}_d\bar{\sigma}^{(0)}][L]^t - [L][{}_d\bar{\sigma}^{(0)}] + [{}_d\bar{\sigma}^{(0)}]\text{tr}([L]) \quad (5.32)$$

Equation 5.31 is the Maxwell rate constitutive equation for compressible polymeric fluids in contra-variant basis.  $\lambda_1$  is relaxation time,  $\eta_0$  is zero shear rate viscosity and  $\kappa_0$  is second viscosity. If the polymeric fluid is incompressible, then  $\text{tr}([L]) = 0$  and we obtain the following:

$$[{}_d\bar{\sigma}^{(0)}] + \lambda_1[{}_d\bar{\sigma}^{(1)}] = 2\eta_0(\bar{\theta})[\gamma^{(1)}] \quad (5.33)$$

in which  $[{}_d\bar{\sigma}^{(1)}]$  is defined by 5.32 but without the term  $[{}_d\bar{\sigma}^{(0)}]\text{tr}([L])$  as it is zero in this case. 5.33 is the standard Maxwell rate constitutive equation in contra-variant basis for incompressible polymeric fluids in which temperature and temperature gradient effects and the initial stress field in the reference configuration are neglected. 5.31 and 5.33 are also known as *upper convected Maxwell rate constitutive equations*.

#### Co-variant basis:

In this case we consider

$$[{}_d\bar{\sigma}_{(1)}] = \sigma_{\alpha_0}[I] + \sigma_{\alpha_1}[{}_d\bar{\sigma}_{(0)}] + \sigma_{\alpha_2}[\gamma_{(1)}] \quad (5.34)$$

The coefficients  $\sigma_{\alpha_i}$  ;  $i = 0, 1, 2$  are functions of  $i_{{}_d\bar{\sigma}_{(0)}} = \text{tr}([{}_d\bar{\sigma}_{(0)}])$  and  $i_{\gamma_{(1)}} = \text{tr}([\gamma_{(1)}])$ , i.e., the first principal invariants of the tensors  $[{}_d\bar{\sigma}_{(0)}]$  and  $[\gamma_{(1)}]$ , density  $\bar{\rho}$  and temperature  $\bar{\theta}$ . Following the procedure used for the contra-variant case we can derive the following (parallel to 5.27).

$$[{}_d\bar{\sigma}_{(1)}] = \bar{\sigma}_0[I] + \underline{A}_1\text{tr}([{}_d\bar{\sigma}_{(0)}])[I] + \underline{A}_2\text{tr}([\gamma_{(1)}])[I] + \underline{A}_3[{}_d\bar{\sigma}_{(0)}] + \underline{A}_4[\gamma_{(1)}] - \underline{A}_5\bar{\theta}[I] \quad (5.35)$$

in which

$$\begin{aligned} \bar{\sigma}_0 &= \sigma_{\alpha_0} \Big|_{\text{ref}} \quad ; \quad \underline{A}_1(\bar{\rho}, \bar{\theta}) = \frac{\partial(\sigma_{\alpha_0})}{\partial(i_{{}_d\bar{\sigma}_{(0)}})} \Big|_{\text{ref}} \quad ; \quad \underline{A}_2(\bar{\rho}, \bar{\theta}) = \frac{\partial(\sigma_{\alpha_0})}{\partial(i_{\gamma_{(1)}})} \Big|_{\text{ref}} \\ \underline{A}_3(\bar{\rho}, \bar{\theta}) &= \sigma_{\alpha_1} \Big|_{\text{ref}} \quad ; \quad \underline{A}_4(\bar{\rho}, \bar{\theta}) = \sigma_{\alpha_2} \Big|_{\text{ref}} \quad ; \quad \underline{A}_5(\bar{\rho}, \bar{\theta}) = -\frac{\partial(\sigma_{\alpha_0})}{\partial\bar{\theta}} \Big|_{\text{ref}} \end{aligned} \quad (5.36)$$

Expression 5.35 is the most general form of linear rate constitutive equation for polymeric fluids (compressible) in co-variant basis based on the rate constitutive theory of orders one in stress and strain rates, i.e.,  $m = 1$  and  $n = 1$ .

From 5.35 we can derive Maxwell rate constitutive equations in co-variant basis. If  $\bar{\sigma}_0 = 0$  (initial configuration is stress free),  $\underline{A}_1 = 0$  and  $\underline{A}_5 = 0$  (no uniform temperature change between configurations) then

$$[{}_d\bar{\sigma}_{(1)}] = \underline{A}_2\text{tr}([\gamma_{(1)}])[I] + \underline{A}_3[{}_d\bar{\sigma}_{(0)}] + \underline{A}_4[\gamma_{(1)}] \quad (5.37)$$

If we define

$$\lambda_1 = -\frac{1}{\underline{A}_3} \quad ; \quad 2\eta_0(\bar{\theta}) = -\frac{\underline{A}_4}{\underline{A}_3} \quad ; \quad \kappa_0(\bar{\theta}) = -\frac{\underline{A}_2}{\underline{A}_3} \quad (5.38)$$

then from 5.37 we obtain

$$[{}_d\bar{\sigma}_{(0)}] + \lambda_1[{}_d\bar{\sigma}_{(1)}] = 2\eta_0(\bar{\theta})[\gamma_{(1)}] + \kappa_0(\bar{\theta}) \text{tr}([\gamma_{(1)}])[I] \quad (5.39)$$

in which (see reference [14])

$$[{}_d\bar{\sigma}_{(1)}] = \frac{D}{Dt}[{}_d\bar{\sigma}_{(0)}] + [{}_d\bar{\sigma}_{(0)}][L] + [L]^t[{}_d\bar{\sigma}_{(0)}] + [{}_d\bar{\sigma}_{(0)}]\text{tr}([L]) \quad (5.40)$$

Equation 5.39 is the Maxwell rate constitutive equation in co-variant basis for compressible polymeric fluids. If the polymeric fluid is incompressible, then  $\text{tr}([\gamma_{(1)}]) = 0$  and we have the following.

$$[{}_d\bar{\sigma}_{(0)}] + \lambda_1[{}_d\bar{\sigma}_{(1)}] = 2\eta_0(\bar{\theta})[\gamma_{(1)}] \quad (5.41)$$

in which  $[{}_d\bar{\sigma}_{(1)}]$  is defined by 5.40 but without the term  $[{}_d\bar{\sigma}^{(0)}]\text{tr}([L])$  as it is zero in this case. 5.41 is the standard Maxwell rate constitutive equation in co-variant basis for incompressible polymeric fluids without temperature and temperature gradient effects and without initial stress field in the reference configuration. 5.39 and 5.41 are also known as *lower convected Maxwell rate constitutive equations*.

### Giesekus constitutive model

The general derivation presented for the constitutive rate equations of order one in the deviatoric Cauchy stress and strain rates ( $m = 1$  and  $n = 1$ ) also form the basis for deriving Giesekus constitutive model generally used for polymer melts (dense polymers) in which the elastic effects are highly dominant. The Giesekus constitutive model is a non-linear viscoelastic model due to the fact that it contains the generators  $[{}_d\bar{\sigma}^{(0)}]^2$  or  $[{}_d\bar{\sigma}_{(0)}]^2$  in the constitutive equation.

#### Contra-variant basis:

When expressing  $[{}_d\bar{\sigma}^{(1)}]$  as a linear combination of the combined generators of its argument tensors  $[{}_d\bar{\sigma}^{(0)}]$  and  $[\gamma^{(1)}]$ , if we limit this only up to quadratic terms in the two argument tensors, then

$$[{}_d\bar{\sigma}^{(1)}] = \sigma\alpha^0[I] + \sigma\alpha^1[{}_d\bar{\sigma}^{(0)}] + \sigma\alpha^2[\gamma^{(1)}] + \sigma\alpha^3[{}_d\bar{\sigma}^{(0)}]^2 + \sigma\alpha^4[\gamma^{(1)}]^2 + \sigma\alpha^5([{}_d\bar{\sigma}^{(0)}][\gamma^{(1)}] + [\gamma^{(1)}][{}_d\bar{\sigma}^{(0)}]) \quad (5.42)$$

In the derivation of the Giesekus constitutive model we neglect the last three terms in 5.42. Thus we begin with

$$[{}_d\bar{\sigma}^{(1)}] = \sigma\alpha^0[I] + \sigma\alpha^1[{}_d\bar{\sigma}^{(0)}] + \sigma\alpha^2[\gamma^{(1)}] + \sigma\alpha^3[{}_d\bar{\sigma}^{(0)}]^2 \quad (5.43)$$

The second fundamental assumption is that we consider the coefficients  $\sigma\alpha^i$ ;  $i = 0, 1, \dots, 3$  to be functions of the first principal invariants of the tensors  $[{}_d\bar{\sigma}^{(0)}]$ ,  $[\gamma^{(1)}]$  and  $[{}_d\bar{\sigma}^{(0)}]^2$  in addition to density  $\bar{\rho}$  and temperature  $\bar{\theta}$ . Let

$$i_{{}_d\bar{\sigma}^{(0)}} = \text{tr}([{}_d\bar{\sigma}^{(0)}]) \quad ; \quad i_{\gamma^{(1)}} = \text{tr}([\gamma^{(1)}]) \quad ; \quad i_{({}_d\bar{\sigma}^{(0)})^2} = i i_{{}_d\bar{\sigma}^{(0)}} = \text{tr}([{}_d\bar{\sigma}^{(0)}]^2) \quad (5.44)$$

We expand  $\sigma\alpha^i$ ;  $i = 0, 1, \dots, 3$  in Taylor series about the reference configuration and retain only up to linear terms in the invariants 5.44 and temperature  $\bar{\theta}$ , and noting that the invariants 5.44 are zero in the reference configuration, we can write

$$\begin{aligned} \sigma\alpha^i &= \sigma\alpha^i \Big|_{\text{ref}} + \frac{\partial(\sigma\alpha^i)}{\partial(i_{{}_d\bar{\sigma}^{(0)}})} \Big|_{\text{ref}} \text{tr}([{}_d\bar{\sigma}^{(0)}]) + \frac{\partial(\sigma\alpha^i)}{\partial(i_{\gamma^{(1)}})} \Big|_{\text{ref}} \text{tr}([\gamma^{(1)}]) + \frac{\partial(\sigma\alpha^i)}{\partial(i_{({}_d\bar{\sigma}^{(0)})^2})} \Big|_{\text{ref}} \text{tr}([{}_d\bar{\sigma}^{(0)}]^2) \\ &\quad + \frac{\partial(\sigma\alpha^i)}{\partial\bar{\theta}} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 0, 1, \dots, 3 \end{aligned} \quad (5.45)$$

Substituting from 5.45 into 5.43 and using  $\varrho = \bar{\theta} - \theta_0$  then we obtain

$$\begin{aligned}
[d\bar{\sigma}^{(1)}] = & \left( \sigma_{\alpha^0} \Big|_{\text{ref}} + \frac{\partial(\sigma_{\alpha^0})}{\partial(i_{d\bar{\sigma}^{(0)}})} \Big|_{\text{ref}} \text{tr}([d\bar{\sigma}^{(0)}]) + \frac{\partial(\sigma_{\alpha^0})}{\partial(i_{\gamma^{(1)}})} \Big|_{\text{ref}} \text{tr}([\gamma^{(1)}]) + \frac{\partial(\sigma_{\alpha^0})}{\partial(i_{(d\bar{\sigma}^{(0)})^2})} \Big|_{\text{ref}} \text{tr}([d\bar{\sigma}^{(0)}]^2) \right. \\
& + \frac{\partial(\sigma_{\alpha^0})}{\partial\bar{\theta}} \Big|_{\text{ref}} \tilde{\theta} \Big) [I] + \left( \sigma_{\alpha^1} \Big|_{\text{ref}} + \frac{\partial(\sigma_{\alpha^1})}{\partial(i_{d\bar{\sigma}^{(0)}})} \Big|_{\text{ref}} \text{tr}([d\bar{\sigma}^{(0)}]) + \frac{\partial(\sigma_{\alpha^1})}{\partial(i_{\gamma^{(1)}})} \Big|_{\text{ref}} \text{tr}([\gamma^{(1)}]) \right. \\
& + \frac{\partial(\sigma_{\alpha^1})}{\partial(i_{(d\bar{\sigma}^{(0)})^2})} \Big|_{\text{ref}} \text{tr}([d\bar{\sigma}^{(0)}]^2) + \frac{\partial(\sigma_{\alpha^1})}{\partial\bar{\theta}} \Big|_{\text{ref}} \tilde{\theta} \Big) [d\bar{\sigma}^{(0)}] + \left( \sigma_{\alpha^2} \Big|_{\text{ref}} + \frac{\partial(\sigma_{\alpha^2})}{\partial(i_{d\bar{\sigma}^{(0)}})} \Big|_{\text{ref}} \text{tr}([d\bar{\sigma}^{(0)}]) \right. \\
& + \frac{\partial(\sigma_{\alpha^2})}{\partial(i_{\gamma^{(1)}})} \Big|_{\text{ref}} \text{tr}([\gamma^{(1)}]) + \frac{\partial(\sigma_{\alpha^2})}{\partial(i_{(d\bar{\sigma}^{(0)})^2})} \Big|_{\text{ref}} \text{tr}([d\bar{\sigma}^{(0)}]^2) + \frac{\partial(\sigma_{\alpha^2})}{\partial\bar{\theta}} \Big|_{\text{ref}} \tilde{\theta} \Big) [\gamma^{(1)}] \\
& + \left( \sigma_{\alpha^3} \Big|_{\text{ref}} + \frac{\partial(\sigma_{\alpha^3})}{\partial(i_{d\bar{\sigma}^{(0)}})} \Big|_{\text{ref}} \text{tr}([d\bar{\sigma}^{(0)}]) + \frac{\partial(\sigma_{\alpha^3})}{\partial(i_{\gamma^{(1)}})} \Big|_{\text{ref}} \text{tr}([\gamma^{(1)}]) + \frac{\partial(\sigma_{\alpha^3})}{\partial(i_{(d\bar{\sigma}^{(0)})^2})} \Big|_{\text{ref}} \text{tr}([d\bar{\sigma}^{(0)}]^2) \right. \\
& \left. + \frac{\partial(\sigma_{\alpha^3})}{\partial\bar{\theta}} \Big|_{\text{ref}} \tilde{\theta} \Big) [d\bar{\sigma}^{(0)}]^2
\end{aligned} \tag{5.46}$$

Neglecting the terms containing products and squares etc. of the generators and invariants, 5.46 reduces to the following:

$$\begin{aligned}
[d\bar{\sigma}^{(1)}] = & \left( \sigma_{\alpha^0} \Big|_{\text{ref}} + \frac{\partial(\sigma_{\alpha^0})}{\partial(i_{d\bar{\sigma}^{(0)}})} \Big|_{\text{ref}} \text{tr}([d\bar{\sigma}^{(0)}]) + \frac{\partial(\sigma_{\alpha^0})}{\partial(i_{\gamma^{(1)}})} \Big|_{\text{ref}} \text{tr}([\gamma^{(1)}]) + \frac{\partial(\sigma_{\alpha^0})}{\partial(i_{(d\bar{\sigma}^{(0)})^2})} \Big|_{\text{ref}} \text{tr}([d\bar{\sigma}^{(0)}]^2) \right. \\
& \left. + \frac{\partial(\sigma_{\alpha^0})}{\partial\bar{\theta}} \Big|_{\text{ref}} \tilde{\theta} \right) [I] + \sigma_{\alpha^1} \Big|_{\text{ref}} [d\bar{\sigma}^{(0)}] + \sigma_{\alpha^2} \Big|_{\text{ref}} [\gamma^{(1)}] + \sigma_{\alpha^3} \Big|_{\text{ref}} [d\bar{\sigma}^{(0)}]^2
\end{aligned} \tag{5.47}$$

Let us define

$$\tilde{A}_1 = \frac{\partial(\sigma_{\alpha^0})}{\partial(i_{d\bar{\sigma}^{(0)}})} \Big|_{\text{ref}} \quad ; \quad \tilde{A}_2 = \frac{\partial(\sigma_{\alpha^0})}{\partial(i_{\gamma^{(1)}})} \Big|_{\text{ref}} \quad ; \quad \tilde{A}_3 = \frac{\partial(\sigma_{\alpha^0})}{\partial(i_{(d\bar{\sigma}^{(0)})^2})} \Big|_{\text{ref}} \quad ; \quad \tilde{A}_4 = -\frac{\partial(\sigma_{\alpha^0})}{\partial\bar{\theta}} \Big|_{\text{ref}} \tag{5.48}$$

Then 5.47 can be written as

$$\begin{aligned}
[d\bar{\sigma}^{(1)}] = & \left( \sigma_{\alpha^0} \Big|_{\text{ref}} + \tilde{A}_1 \text{tr}([d\bar{\sigma}^{(0)}]) + \tilde{A}_2 \text{tr}([\gamma^{(1)}]) + \tilde{A}_3 \text{tr}([d\bar{\sigma}^{(0)}]^2) - \tilde{A}_4 \tilde{\theta} \right) [I] \\
& + \sigma_{\alpha^1} \Big|_{\text{ref}} [d\bar{\sigma}^{(0)}] + \sigma_{\alpha^2} \Big|_{\text{ref}} [\gamma^{(1)}] + \sigma_{\alpha^3} \Big|_{\text{ref}} [d\bar{\sigma}^{(0)}]^2
\end{aligned} \tag{5.49}$$

If we assume  $\sigma_{\alpha^0} \Big|_{\text{ref}} = 0$  (no initial stress field in the reference configuration) and  $\tilde{A}_1 = \tilde{A}_3 = \tilde{A}_4 = 0$  then 5.49 reduces to

$$[d\bar{\sigma}^{(1)}] = \sigma_{\alpha^1} \Big|_{\text{ref}} [d\bar{\sigma}^{(0)}] + \sigma_{\alpha^2} \Big|_{\text{ref}} [\gamma^{(1)}] + \sigma_{\alpha^3} \Big|_{\text{ref}} [d\bar{\sigma}^{(0)}]^2 + \tilde{A}_2 \text{tr}([\gamma^{(1)}]) [I] \tag{5.50}$$

Terms in 5.50 can be rearranged and if we define the following new constants

$$d_1 = -\frac{1}{\sigma_{\alpha^1} \Big|_{\text{ref}}} \quad ; \quad d_2 = -\frac{\sigma_{\alpha^3} \Big|_{\text{ref}}}{\sigma_{\alpha^1} \Big|_{\text{ref}}} \quad ; \quad d_3 = -\frac{\sigma_{\alpha^2} \Big|_{\text{ref}}}{\sigma_{\alpha^1} \Big|_{\text{ref}}} \quad ; \quad d_4 = -\frac{\tilde{A}_2}{\sigma_{\alpha^1} \Big|_{\text{ref}}} \tag{5.51}$$

then 5.50 can be written as

$$[d\bar{\sigma}^{(0)}] + d_1 [d\bar{\sigma}^{(1)}] - d_2 [d\bar{\sigma}^{(0)}]^2 = d_3 [\gamma^{(1)}] + d_4 \text{tr}([\gamma^{(1)}]) [I] \tag{5.52}$$

To introduce the commonly used notation we define

$$\begin{aligned}\lambda_1 &= d_1 \quad ; \quad \text{relaxation time} \\ 2\eta(\bar{\theta}) &= d_3 \quad ; \quad \eta(\bar{\theta}) \text{ being total viscosity (at zero shear rate)} \\ \kappa(\bar{\theta}) &= d_4 \quad ; \quad \text{second viscosity (at zero shear rate)}\end{aligned}$$

We note that 5.52 is a constitutive equation for the deviatoric stress  $[_d\bar{\sigma}^{(0)}]$  and  $d_2$  is multiplied with  $[_d\bar{\sigma}^{(0)}]^2$ . Thus  $d_2$  must have dimensions of (1/stress) which is the same as (time/dimension of viscosity), i.e.,  $\frac{\lambda_1}{\eta}$ . We choose

$$d_2 = \frac{\lambda_1}{\eta} \alpha$$

$\alpha$  being a dimensionless parameter called mobility factor. Thus 5.52 can be written as

$$[_d\bar{\sigma}^{(0)}] + \lambda_1 [_d\bar{\sigma}^{(1)}] - \frac{\lambda_1}{\eta} \alpha [_d\bar{\sigma}^{(0)}]^2 = 2\eta[\gamma^{(1)}] + \kappa \text{tr}([\gamma^{(1)}])[I] \quad (5.53)$$

where  $[_d\bar{\sigma}^{(1)}]$  has already been defined for the compressible case. 5.53 is the constitutive model for compressible Giesekus fluids in contra-variant basis in contra-variant deviatoric Cauchy stress.  $\kappa$  is the second viscosity. If the polymeric fluid is incompressible then  $\text{tr}([\gamma^{(1)}]) = 0$  and we obtain the following:

$$[_d\bar{\sigma}^{(0)}] + \lambda_1 [_d\bar{\sigma}^{(1)}] - \frac{\lambda_1}{\eta} \alpha [_d\bar{\sigma}^{(0)}]^2 = 2\eta[\gamma^{(1)}] \quad (5.54)$$

Definition of  $[_d\bar{\sigma}^{(1)}]$  for the incompressible case has also been given earlier. 5.54 is the most common form of Giesekus constitutive model for incompressible dense polymeric liquids in which temperature and temperature gradient effects are neglected. 5.54 is also known as *upper convected Giesekus rate constitutive model*.

### Co-variant basis:

To derive Giesekus constitutive model in co-variant basis we begin with (parallel to 5.43 used for contra-variant basis)

$$[_d\bar{\sigma}_{(1)}] = \sigma_{\alpha_0}[I] + \sigma_{\alpha_1}[_d\bar{\sigma}_{(0)}] + \sigma_{\alpha_2}[\gamma_{(1)}] + \sigma_{\alpha_3}[_d\bar{\sigma}_{(0)}]^2 \quad (5.55)$$

The coefficients  $\sigma_{\alpha_i}$  ;  $i = 0, 1, 2, 3$  are assumed to be functions of the first invariants of the tensors  $[_d\bar{\sigma}_{(0)}]$ ,  $[\gamma_{(1)}]$  and  $[_d\bar{\sigma}_{(0)}]^2$  in addition to density  $\bar{\rho}$  and temperature  $\bar{\theta}$ . Let

$$i_{_d\bar{\sigma}_{(0)}} = \text{tr}([_d\bar{\sigma}_{(0)}]) \quad ; \quad i_{\gamma_{(1)}} = \text{tr}([\gamma_{(1)}]) \quad ; \quad i_{(_d\bar{\sigma}_{(0)})^2} = i_{i_{_d\bar{\sigma}_{(0)}}} = \text{tr}([_d\bar{\sigma}_{(0)}]^2) \quad (5.56)$$

Following the procedure used for the contra-variant case we can derive the following:

$$\begin{aligned}[_d\bar{\sigma}_{(1)}] &= \left( \sigma_{\alpha_0} \Big|_{\text{ref}} + \underline{A}_1 \text{tr}([_d\bar{\sigma}_{(0)}]) + \underline{A}_2 \text{tr}([\gamma_{(1)}]) + \underline{A}_3 \text{tr}([_d\bar{\sigma}_{(0)}]^2) - \underline{A}_4 \bar{\theta} \right) [I] \\ &+ \sigma_{\alpha_1} \Big|_{\text{ref}} [_d\bar{\sigma}_{(0)}] + \sigma_{\alpha_2} \Big|_{\text{ref}} [\gamma_{(1)}] + \sigma_{\alpha_3} \Big|_{\text{ref}} [_d\bar{\sigma}_{(0)}]^2\end{aligned} \quad (5.57)$$

where

$$\underline{A}_1 = \frac{\partial(\sigma_{\alpha_0})}{\partial(i_{_d\bar{\sigma}_{(0)}})} \Big|_{\text{ref}} \quad ; \quad \underline{A}_2 = \frac{\partial(\sigma_{\alpha_0})}{\partial(i_{\gamma_{(1)}})} \Big|_{\text{ref}} \quad ; \quad \underline{A}_3 = \frac{\partial(\sigma_{\alpha_0})}{\partial(i_{(_d\bar{\sigma}_{(0)})^2})} \Big|_{\text{ref}} \quad ; \quad \underline{A}_4 = -\frac{\partial(\sigma_{\alpha_0})}{\partial\bar{\theta}} \Big|_{\text{ref}} \quad (5.58)$$

If we assume that  $\sigma_{\alpha_0}|_{\text{ref}} = 0$  (no initial stress field in the reference configuration) and  $\underline{A}_1 = \underline{A}_3 = \underline{A}_4 = 0$ , then 5.57 reduces to

$$[_d\bar{\sigma}_{(1)}] = \sigma_{\alpha_1} \Big|_{\text{ref}} [_d\bar{\sigma}_{(0)}] + \sigma_{\alpha_2} \Big|_{\text{ref}} [\gamma_{(1)}] + \sigma_{\alpha_3} \Big|_{\text{ref}} [_d\bar{\sigma}_{(0)}]^2 + \underline{A}_2 \text{tr}([\gamma_{(1)}])[I] \quad (5.59)$$

If we define the following new constants

$$\underline{d}_1 = -\frac{1}{\sigma_{\alpha_1}|_{\text{ref}}} \quad ; \quad \underline{d}_2 = -\frac{\sigma_{\alpha_3}|_{\text{ref}}}{\sigma_{\alpha_1}|_{\text{ref}}} \quad ; \quad \underline{d}_3 = -\frac{\sigma_{\alpha_2}|_{\text{ref}}}{\sigma_{\alpha_1}|_{\text{ref}}} \quad ; \quad \underline{d}_4 = -\frac{\tilde{A}_2}{\sigma_{\alpha_1}|_{\text{ref}}} \quad (5.60)$$

then terms in 5.59 can be rearranged giving the following:

$$[{}_d\bar{\sigma}_{(0)}] + \underline{d}_1[{}_d\bar{\sigma}_{(1)}] - \underline{d}_2[{}_d\bar{\sigma}_{(0)}]^2 = \underline{d}_3[\gamma_{(1)}] + \underline{d}_4\text{tr}([\gamma_{(1)}])[I] \quad (5.61)$$

To introduce the commonly used notation we define

$$\lambda_1 = \underline{d}_1 \quad ; \quad \text{relaxation time}$$

$$2\eta(\bar{\theta}) = \underline{d}_3 \quad ; \quad \eta(\bar{\theta}) \text{ being total viscosity}$$

$$\kappa(\bar{\theta}) = \underline{d}_4 \quad ; \quad \text{second viscosity}$$

We note that 5.61 is a constitutive equation for the deviatoric stress  $[{}_d\bar{\sigma}_{(0)}]$  and  $\underline{d}_2$  is multiplied with  $[{}_d\bar{\sigma}_{(0)}]^2$ . Thus  $\underline{d}_2$  must have dimensions of (1/stress) which is the same as (time/dimension of viscosity), i.e.,  $\frac{\lambda_1}{\eta}$ . We choose

$$\underline{d}_2 = \frac{\lambda_1}{\eta} \alpha$$

$\alpha$  being a dimensionless parameter called mobility factor. Thus 5.61 can be written as

$$[{}_d\bar{\sigma}_{(0)}] + \lambda_1[{}_d\bar{\sigma}_{(1)}] - \frac{\lambda_1}{\eta} \alpha [{}_d\bar{\sigma}_{(0)}]^2 = 2\eta[\gamma_{(1)}] + \kappa \text{tr}([\gamma_{(1)}])[I] \quad (5.62)$$

where  $[{}_d\bar{\sigma}_{(1)}]$  has already been defined for the compressible case. 5.62 is the constitutive model for compressible Giesekus fluids in co-variant basis in contra-variant deviatoric Cauchy stress.  $\kappa$  is the second viscosity. If the polymeric fluid is incompressible then  $\text{tr}([\gamma_{(1)}]) = 0$  and we obtain the following:

$$[{}_d\bar{\sigma}_{(0)}] + \lambda_1[{}_d\bar{\sigma}_{(1)}] - \frac{\lambda_1}{\eta} \alpha [{}_d\bar{\sigma}_{(0)}]^2 = 2\eta[\gamma_{(1)}] \quad (5.63)$$

Definition of  $[{}_d\bar{\sigma}_{(1)}]$  for the incompressible case has also been given earlier. 5.63 is the most general form of Giesekus constitutive model for incompressible dense polymeric liquids in which temperature and temperature gradient effects are neglected. 5.63 is also known as *lower convected Giesekus rate constitutive model*.

## 5.5 Rate constitutive equations of order one in deviatoric Cauchy stress rate and of order two in strain rate

We consider rate constitutive equations of order one in deviatoric Cauchy stress rate and order two in strain rate, i.e.,  $m = 1$  and  $n = 2$ . This forms the basis for deriving Oldroyd-B model.

### Contra-variant basis:

In the absence of  $\bar{\mathbf{g}}$  as an argument tensor but permitting uniform temperature change from the reference to the current configuration, we have the following for the first convected time derivative of the deviatoric Cauchy stress tensor in contra-variant basis.

$$[{}_d\bar{\sigma}^{(1)}] = [{}_d\bar{\sigma}^{(1)}(\bar{\rho}, [{}_d\bar{\sigma}^{(0)}], [\gamma^{(1)}], [\gamma^{(2)}], \bar{\theta})] \quad (5.64)$$

The development of the constitutive theory in this case requires: (i) combined generators of  $[{}_d\bar{\sigma}^{(0)}]$ ,  $[\gamma^{(1)}]$  and  $[\gamma^{(2)}]$  (symmetric tensors of rank two) that are also symmetric tensors of rank two due to the fact that  $[{}_d\bar{\sigma}^{(1)}]$

is a symmetric tensor of rank two (ii) combined invariants of the tensors  $[d\bar{\sigma}^{(0)}]$ ,  $[\gamma^{(1)}]$  and  $[\gamma^{(2)}]$ . We express  $[d\bar{\sigma}^{(1)}]$  as a linear combination of  $[I]$  and the combined generators.

$$[d\bar{\sigma}^{(1)}] = \sigma_{\alpha^0}[I] + \sum_{i=1}^{n^*} \sigma_{\alpha^i}[\sigma \tilde{G}^i] \quad (5.65)$$

in which  $[\sigma \tilde{G}^i]$ ;  $i = 1, 2, \dots, n^*$  are the combined generators. The coefficients  $\sigma_{\alpha^i}$ ;  $i = 0, 1, \dots, n^*$  are functions of the combined generators  $\sigma \tilde{I}^j$ ;  $j = 1, 2, \dots, m^*$ , density  $\bar{\rho}$  and temperature  $\bar{\theta}$  and are determined by using Taylor series expansion of each  $\sigma_{\alpha^i}$  about the reference configuration and only retaining up to the linear terms in the combined invariants and temperature. When these coefficients are substituted back into 5.65, we have the final form of the constitutive equations of order one in stress rate and of order two in strain rate (similar to 5.15). Details are straight forward hence are omitted.

### Co-variant basis:

In the absence of  $\bar{\mathbf{g}}$  as an argument tensor but permitting uniform temperature change from the reference to the current configuration, in co-variant basis we have

$$[d\bar{\sigma}_{(1)}] = [d\bar{\sigma}_{(1)}(\bar{\rho}, [d\bar{\sigma}_{(0)}], [\gamma_{(1)}], [\gamma_{(2)}], \bar{\theta})] \quad (5.66)$$

If  $[\sigma \tilde{G}_i]$ ;  $i = 1, 2, \dots, n^*$  and  $\sigma \tilde{I}_i$ ;  $i = 1, 2, \dots, m^*$  are combined generators (symmetric tensors of order two) and invariants of the symmetric tensors  $[d\bar{\sigma}_{(0)}]$ ,  $[\gamma_{(1)}]$  and  $[\gamma_{(2)}]$  of rank two then

$$[d\bar{\sigma}_{(1)}] = \sigma_{\alpha_0}[I] + \sum_{i=1}^{n^*} \sigma_{\alpha_i}[\sigma \tilde{G}_i] \quad (5.67)$$

Remaining details follow the contra-variant derivation hence are omitted.

### Oldroyd-B constitutive model

Oldroyd-B constitutive model is a special case of the rate constitutive equations that are of order one in deviatoric Cauchy stress rate and of order two in strain rate. This model is also referred to as quasi-nonlinear constitutive model [5]. Derivation of this constitutive model in contra-variant and co-variant bases is given in the following.

### Contra-variant basis:

We express  $[d\bar{\sigma}^{(1)}]$  as a linear combination of  $[I]$  and the generators  $[d\bar{\sigma}^{(0)}]$ ,  $[\gamma^{(1)}]$  and  $[\gamma^{(2)}]$  only out of the combined generators of the tensors  $[d\bar{\sigma}^{(0)}]$ ,  $[\gamma^{(1)}]$  and  $[\gamma^{(2)}]$ .

$$[d\bar{\sigma}^{(1)}] = \sigma_{\alpha^0}[I] + \sigma_{\alpha^1}[d\bar{\sigma}^{(0)}] + \sigma_{\alpha^2}[\gamma^{(1)}] + \sigma_{\alpha^3}[\gamma^{(2)}] \quad (5.68)$$

We further assume that the coefficients  $\sigma_{\alpha^i}$ ;  $i = 0, 1, \dots, 3$  only depend upon the first invariants of the tensors  $[d\bar{\sigma}^{(0)}]$ ,  $[\gamma^{(1)}]$  and  $[\gamma^{(2)}]$  in addition to density  $\bar{\rho}$  and temperature  $\bar{\theta}$ . Let

$$i_{d\bar{\sigma}^{(0)}} = \text{tr}([d\bar{\sigma}^{(0)}]) \quad ; \quad i_{\gamma^{(1)}} = \text{tr}([\gamma^{(1)}]) \quad ; \quad i_{\gamma^{(2)}} = \text{tr}([\gamma^{(2)}]) \quad (5.69)$$

We expand  $\sigma_{\alpha^i}$ ;  $i = 0, 1, \dots, 3$  in Taylor series about the reference configuration and retain only up to the first order terms in the invariants 5.69 and temperature  $\bar{\theta}$ , and noting that the invariants 5.69 in the reference configuration are all zero, we can write

$$\begin{aligned} \sigma_{\alpha^i} = & \sigma_{\alpha^i} \Big|_{\text{ref}} + \frac{\partial(\sigma_{\alpha^i})}{\partial(i_{d\bar{\sigma}^{(0)}})} \Big|_{\text{ref}} \text{tr}([d\bar{\sigma}^{(0)}]) + \frac{\partial(\sigma_{\alpha^i})}{\partial(i_{\gamma^{(1)}})} \Big|_{\text{ref}} \text{tr}([\gamma^{(1)}]) + \frac{\partial(\sigma_{\alpha^i})}{\partial(i_{\gamma^{(2)}})} \Big|_{\text{ref}} \text{tr}([\gamma^{(2)}]) \\ & + \frac{\partial(\sigma_{\alpha^i})}{\partial\bar{\theta}} \Big|_{\text{ref}} \bar{\theta} \quad ; \quad i = 0, 1, \dots, 3 \end{aligned} \quad (5.70)$$

where  $\tilde{\theta} = \bar{\theta} - \theta_0$ . Substituting from 5.70 into 5.68 and neglecting products of  $\text{tr}([d\bar{\sigma}^{(0)}])$ ,  $\text{tr}([\gamma^{(1)}])$ ,  $\text{tr}([\gamma^{(2)}])$  and  $\tilde{\theta}$  with  $[d\bar{\sigma}^{(0)}]$ ,  $[\gamma^{(1)}]$  and  $[\gamma^{(2)}]$

$$[d\bar{\sigma}^{(1)}] = \left( \sigma_{\alpha^0} \Big|_{\text{ref}} + \frac{\partial(\sigma_{\alpha^0})}{\partial(i_{d\bar{\sigma}^{(0)}})} \Big|_{\text{ref}} \text{tr}([d\bar{\sigma}^{(0)}]) + \frac{\partial(\sigma_{\alpha^0})}{\partial(i_{\gamma^{(1)}})} \Big|_{\text{ref}} \text{tr}([\gamma^{(1)}]) + \frac{\partial(\sigma_{\alpha^0})}{\partial(i_{\gamma^{(2)}})} \Big|_{\text{ref}} \text{tr}([\gamma^{(2)}]) \right. \\ \left. + \frac{\partial(\sigma_{\alpha^0})}{\partial\theta} \Big|_{\text{ref}} \tilde{\theta} \right) [I] + \sigma_{\alpha^1} \Big|_{\text{ref}} [d\bar{\sigma}^{(0)}] + \sigma_{\alpha^2} \Big|_{\text{ref}} [\gamma^{(1)}] + \sigma_{\alpha^3} \Big|_{\text{ref}} [\gamma^{(2)}] \quad (5.71)$$

Let us define

$$\tilde{A}_1 = \frac{\partial(\sigma_{\alpha^0})}{\partial(i_{d\bar{\sigma}^{(0)}})} \Big|_{\text{ref}} ; \quad \tilde{A}_2 = \frac{\partial(\sigma_{\alpha^0})}{\partial(i_{\gamma^{(1)}})} \Big|_{\text{ref}} ; \quad \tilde{A}_3 = \frac{\partial(\sigma_{\alpha^0})}{\partial(i_{\gamma^{(2)}})} \Big|_{\text{ref}} ; \quad \tilde{A}_4 = -\frac{\partial(\sigma_{\alpha^0})}{\partial\theta} \Big|_{\text{ref}} \quad (5.72)$$

then 5.71 can be written as

$$[d\bar{\sigma}^{(1)}] = \left( \sigma_{\alpha^0} \Big|_{\text{ref}} + \tilde{A}_1 \text{tr}([d\bar{\sigma}^{(0)}]) + \tilde{A}_2 \text{tr}([\gamma^{(1)}]) + \tilde{A}_3 \text{tr}([\gamma^{(2)}]) - \tilde{A}_4 \tilde{\theta} \right) [I] + \sigma_{\alpha^1} \Big|_{\text{ref}} [d\bar{\sigma}^{(0)}] \\ + \sigma_{\alpha^2} \Big|_{\text{ref}} [\gamma^{(1)}] + \sigma_{\alpha^3} \Big|_{\text{ref}} [\gamma^{(2)}] \quad (5.73)$$

In order to derive Oldroyd-B model from 5.73 we assume  $\sigma_{\alpha^0} \Big|_{\text{ref}} = 0$  in addition to  $\tilde{A}_1 = 0$  and  $\tilde{A}_4 = 0$ . Dividing 5.73 by  $\sigma_{\alpha^1} \Big|_{\text{ref}}$  and introducing the following new constants

$$\lambda_1 = -\frac{1}{\sigma_{\alpha^1} \Big|_{\text{ref}}} ; \quad 2\eta(\bar{\theta}) = -\frac{\sigma_{\alpha^2} \Big|_{\text{ref}}}{\sigma_{\alpha^1} \Big|_{\text{ref}}} ; \quad \beta_1(\bar{\theta}) = -\frac{\sigma_{\alpha^3} \Big|_{\text{ref}}}{\sigma_{\alpha^1} \Big|_{\text{ref}}} ; \quad \kappa(\bar{\theta}) = -\frac{\tilde{A}_2}{\sigma_{\alpha^1} \Big|_{\text{ref}}} ; \quad \kappa_2(\bar{\theta}) = -\frac{\tilde{A}_3}{\sigma_{\alpha^1} \Big|_{\text{ref}}} \quad (5.74)$$

where  $\eta$  is the zero shear rate viscosity,  $\kappa$  is the second viscosity and  $\lambda_1$  is the relaxation time, we obtain

$$[d\bar{\sigma}^{(0)}] + \lambda_1 [d\bar{\sigma}^{(1)}] = 2\eta[\gamma^{(1)}] + \beta_1[\gamma^{(2)}] + \kappa \text{tr}([\gamma^{(1)}])[I] + \kappa_2 \text{tr}([\gamma^{(2)}])[I] \quad (5.75)$$

We note that  $[\gamma^{(1)}]$  and  $[\gamma^{(2)}]$  are first and second convected time derivatives of the Almansi strain tensor. Thus dimensionally (or in terms of units), if we multiply  $[\gamma^{(2)}]$  by time we obtain the units of  $[\gamma^{(1)}]$ . Since  $[\gamma^{(1)}]$  is multiplied with  $2\eta$ , then  $[\gamma^{(2)}]$  must be multiplied with  $2\eta$  also and a time constant, say  $\lambda_2$ . Thus we can choose  $\beta_1 = 2\eta\lambda_2$  where  $\lambda_2$  is called retardation time. Following the same argument  $\kappa_2$  has similar meaning as  $\kappa$  but must be multiplied with a time constant. Thus we obtain the following from 5.75.

$$[d\bar{\sigma}^{(0)}] + \lambda_1 [d\bar{\sigma}^{(1)}] = 2\eta([\gamma^{(1)}] + \lambda_2 [\gamma^{(2)}]) + \kappa \text{tr}([\gamma^{(1)}])[I] + \kappa_2 \text{tr}([\gamma^{(2)}])[I] \quad (5.76)$$

Expression 5.76 is the constitutive model for compressible Oldroyd-B fluids in contra-variant basis. Definition of  $[d\bar{\sigma}^{(1)}]$  has already been given. If we consider the fluid to be incompressible then  $\text{tr}([\gamma^{(1)}])$  and  $\text{tr}([\gamma^{(2)}])$  are zero and 5.76 for incompressible Oldroyd-B fluids reduces to

$$[d\bar{\sigma}^{(0)}] + \lambda_1 [d\bar{\sigma}^{(1)}] = 2\eta([\gamma^{(1)}] + \lambda_2 [\gamma^{(2)}]) \quad (5.77)$$

We remark that in 5.77, temperature and temperature gradient effects are neglected. 5.76 and 5.77 are also known as *upper convected Oldroyd-B rate constitutive equations*.

### Co-variant basis:

In co-variant basis we consider

$$[d\bar{\sigma}_{(1)}] = \sigma_{\alpha^0} [I] + \sigma_{\alpha^1} [d\bar{\sigma}_{(0)}] + \sigma_{\alpha^2} [\gamma_{(1)}] + \sigma_{\alpha^3} [\gamma_{(2)}] \quad (5.78)$$

Following the procedure and details presented for contra-variant case we can derive

$$[d\bar{\sigma}_{(0)}] + \lambda_1 [d\bar{\sigma}_{(1)}] = 2\eta([\gamma_{(1)}] + \lambda_2 [\gamma_{(2)}]) + \kappa \text{tr}([\gamma_{(1)}])[I] + \kappa_2 \text{tr}([\gamma_{(2)}])[I] \quad (5.79)$$

for compressible Oldroyd-B fluids (neglecting temperature and temperature gradient effects and assuming that the initial configuration is stress free). If we consider the fluid to be incompressible then  $\text{tr}([\gamma_{(1)}])$  and  $\text{tr}([\gamma_{(2)}])$  are zero and 5.79 for incompressible Oldroyd-B fluids reduces to

$$[{}_d\bar{\sigma}_{(0)}] + \lambda_1[{}_d\bar{\sigma}_{(1)}] = 2\eta([\gamma_{(1)}] + \lambda_2[\gamma_{(2)}]) \quad (5.80)$$

Expression 5.80 is Oldroyd-B constitutive model for incompressible fluids. 5.79 and 5.80 are also called *lower convected Oldroyd-B rate constitutive equations*.

## 6 Development of constitutive equations for the heat vector

It has been shown in section 3 that based on the principle of equipresence and physics of deforming fluids we can consider the following argument tensors for the heat vector in contra- and co-variant bases.

### Contra-variant basis:

In this case we have

$$\bar{\mathbf{q}}^{(0)} = \bar{\mathbf{q}}^{(0)}([{}_d\sigma^{(i)}]; i = 0, 1, \dots, m-1, [\gamma^{(j)}]; j = 1, 2, \dots, n, \bar{\theta}, \bar{\mathbf{g}}) \quad (6.1)$$

Here 6.1 holds for compressible fluids. If we consider the fluid to be incompressible then dependence of  $\bar{\mathbf{q}}^{(0)}$  on density  $\bar{\rho}$  drops out in 6.1.

### Co-variant basis:

In this case we have

$$\bar{\mathbf{q}}_{(0)} = \bar{\mathbf{q}}_{(0)}([{}_d\sigma_{(i)}]; i = 0, 1, \dots, m-1, [\gamma_{(j)}]; j = 1, 2, \dots, n, \bar{\theta}, \bar{\mathbf{g}}) \quad (6.2)$$

In this case also, 6.2 holds for compressible fluids. If we assume the fluid to be incompressible, then  $\rho = \bar{\rho}$  and hence density  $\bar{\rho}$  is no longer an argument in 6.2.

In the following two sections we first present a general theory for the constitutive equations for  $\bar{\mathbf{q}}^{(0)}$  and  $\bar{\mathbf{q}}_{(0)}$  that are of orders ‘ $m-1$ ’ in stress rate and ‘ $n$ ’ in strain rate. In subsequent sections this is specialized for Maxwell, Giesekus and Oldroyd-B fluids.

### 6.1 Constitutive equations for heat vector of orders $m-1$ and $n$ in deviatoric Cauchy stress and strain rates

#### Contra-variant basis

Consider 6.1 and its argument tensors. We note that  $[{}_d\sigma^{(i)}]; i = 0, 1, \dots, m-1$  and  $[\gamma^{(j)}]; j = 1, 2, \dots, n$  are symmetric tensors of rank two whereas  $\bar{\mathbf{g}}$  is a tensor of rank one and so is  $\bar{\mathbf{q}}^{(0)}$ . Thus, to express  $\bar{\mathbf{q}}^{(0)}$  in terms of a linear combination of the combined generators  $\{^q\tilde{G}^i\}; i = 1, 2, \dots, N$  of  $[{}_d\sigma^{(i)}]; i = 0, 1, \dots, m-1$ ,  $[\gamma^{(j)}]; j = 1, 2, \dots, n$  and  $\bar{\mathbf{g}}$ ,  $\{^q\tilde{G}^i\}$  must be tensors of rank one. Let  $^q\tilde{I}^j; j = 1, 2, \dots, M$  be the combined invariants of the tensors  $[{}_d\sigma^{(i)}]; i = 0, 1, \dots, m-1$ ,  $[\gamma^{(j)}]; j = 1, 2, \dots, n$  and  $\bar{\mathbf{g}}$ . We can express  $\bar{\mathbf{q}}^{(0)}$  as a linear combination of the combined generators  $\{^q\tilde{G}^i\}$ .

$$\bar{\mathbf{q}}^{(0)} = - \sum_{i=1}^N q_{\alpha}^i \{^q\tilde{G}^i\} \quad (6.3)$$

The coefficients  $q_{\alpha}^i; i = 1, 2, \dots, N$  are functions of the combined invariants  $^q\tilde{I}^j; j = 1, 2, \dots, M$ , density  $\bar{\rho}$  and temperature  $\bar{\theta}$  and are determined by using their Taylor series expansion about the reference configuration and retaining only up to first order terms in the combined invariants  $^q\tilde{I}^j$  and temperature  $\bar{\theta}$ .

$$q_{\alpha}^i = q_{\alpha}^i \Big|_{\text{ref}} + \sum_{j=1}^M \frac{\partial(q_{\alpha}^i)}{\partial(^q\tilde{I}^j)} \Big|_{\text{ref}} (^q\tilde{I}^j - ^q\tilde{I}^j|_{\text{ref}}) + \frac{\partial(q_{\alpha}^i)}{\partial(\bar{\theta})} \Big|_{\text{ref}} (\bar{\theta} - \theta_0) \quad ; \quad i = 0, 1, \dots, N \quad (6.4)$$

In the reference configuration the combined invariants are zero, i.e.,  $\tilde{qI}^j|_{\text{ref}} = 0$  due to stress free, zero velocity and temperature gradient free medium. Hence 6.4 simplifies to

$$q_{\alpha}^i = q_{\alpha}^i \Big|_{\text{ref}} + \sum_{j=1}^M \frac{\partial(q_{\alpha}^i)}{\partial(\tilde{qI}^j)} \Big|_{\text{ref}} \tilde{qI}^j + \frac{\partial(q_{\alpha}^i)}{\partial(\tilde{qI}^j)} \Big|_{\text{ref}} \tilde{\theta} \quad ; \quad i = 0, 1, \dots, N \quad (6.5)$$

where  $\tilde{\theta} = \bar{\theta} - \theta_0$ . By substituting from 6.5 into 6.3 we obtain the most general form of the constitutive equation for heat vectors that are of order ' $m - 1$ ' in stress rate and of order ' $n$ ' in strain rate.

### Co-variant basis

In the co-variant basis, we consider 6.2 and express  $\bar{\mathbf{q}}_{(0)}$  as a linear combination of the combined generators  $\{q_{\alpha}^i\}$ ;  $i = 1, 2, \dots, N$  (tensors of rank one).

$$\bar{\mathbf{q}}_{(0)} = - \sum_{i=1}^N q_{\alpha}^i \{q_{\alpha}^i\} \quad (6.6)$$

The coefficients  $q_{\alpha}^i$ ;  $i = 1, 2, \dots, N$  are functions of the combined invariants  $\tilde{qI}^j$ ;  $j = 1, 2, \dots, M$  of tensors  $[d\sigma_{(i)}]$ ;  $i = 0, 1, \dots, m - 1$ ,  $[\gamma_{(j)}]$ ;  $j = 1, 2, \dots, n$  and  $\bar{\mathbf{g}}$ , as well as density  $\bar{\rho}$  and temperature  $\bar{\theta}$ . Following the procedure presented for contra-variant basis we can derive expressions for  $q_{\alpha}^i$ ;  $i = 1, 2, \dots, N$  (similar to 6.4 and 6.5). Substituting  $q_{\alpha}^i$  into 6.6 gives the constitutive equation for heat vector  $\bar{\mathbf{q}}_{(0)}$  in co-variant basis.

If the fluid is considered to be incompressible then dependence of the coefficients on density  $\bar{\rho}$  is eliminated and incompressibility condition must be imposed through the invariants, but the general derivation remains the same.

## 6.2 Constitutive equations for heat vector of order zero in deviatoric Cauchy stress rate and of order one in strain rate

These constitutive equations in contra-variant and co-variant bases contain the same argument tensors as the rate constitutive equations for deviatoric stress that are of order 1 in stress and strain rates (derived in section 5.4), with  $\bar{\mathbf{g}}$  being an additional argument tensor. We consider

$$\begin{aligned} \bar{\mathbf{q}}^{(0)} &= \bar{\mathbf{q}}^{(0)}(\bar{\rho}, [d\sigma^{(0)}], [\gamma^{(1)}], \bar{\theta}, \bar{\mathbf{g}}) \\ \text{and} \quad \bar{\mathbf{q}}_{(0)} &= \bar{\mathbf{q}}_{(0)}(\bar{\rho}, [d\sigma_{(0)}], [\gamma_{(1)}], \bar{\theta}, \bar{\mathbf{g}}) \end{aligned} \quad (6.7)$$

in contra- and co-variant bases. The derivations follow the previous derivations but utilizing combined generators and the combined invariants of the argument tensors  $[d\sigma^{(0)}]$ ,  $[\gamma^{(1)}]$ ,  $\bar{\mathbf{g}}$  and  $[d\sigma_{(0)}]$ ,  $[\gamma_{(1)}]$ ,  $\bar{\mathbf{g}}$  in contra- and co-variant bases. The dependence of the coefficients in the linear combination are generally limited to the first principal invariants of the argument tensors. The constitutive model for heat vector is suitable for using with Maxwell model for the deviatoric stress. If we only consider the generator of  $\bar{\mathbf{g}}$  as argument of  $\bar{\mathbf{q}}^{(0)}$  and  $\bar{\mathbf{q}}_{(0)}$ , then we obtain the Fourier heat conduction law (see references [14, 26]). The choice of the specific form of the constitutive equation for heat vector is a matter of application and ability to calibrate the constitutive model by determining the coefficients experimentally.

In case of Giesekus constitutive model for the deviatoric stress, the generators  $[d\sigma^{(0)}]$ ,  $[\gamma^{(1)}]$ , and  $[d\sigma^{(0)}]^2$  (and their counterpart in co-variant basis) are used in defining the first convected time derivative of Cauchy stress tensor, i.e.,  $[d\sigma^{(1)}]$ . Use of  $[d\sigma^{(0)}]^2$  for  $\bar{\mathbf{q}}^{(0)}$  unnecessarily complicates the derivation and increases the necessity for determining more coefficients experimentally. Use of the same constitutive model for the heat vector as described for Maxwell fluids is justified in this case also. Generally the use of Fourier heat conduction law is the most commonly used practice.

### 6.3 Constitutive equations for heat vector of order zero in stress rate and of order two in strain rate

In this case we consider

$$\begin{aligned}\bar{\mathbf{q}}^{(0)} &= \bar{\mathbf{q}}^{(0)}(\bar{\rho}, [d\sigma^{(0)}], [\gamma^{(1)}], [\gamma^{(2)}], \bar{\theta}, \bar{\mathbf{g}}) \\ \text{and} \quad \bar{\mathbf{q}}_{(0)} &= \bar{\mathbf{q}}_{(0)}(\bar{\rho}, [d\sigma_{(0)}], [\gamma_{(1)}], [\gamma_{(2)}], \bar{\theta}, \bar{\mathbf{g}})\end{aligned}\tag{6.8}$$

in contra- and co-variant bases. Details of the derivations follow previous cases and hence are omitted. If we impose the same restriction on the determination of the coefficients as used in the case of the constitutive equation for Oldroyd-B fluids, then we obtain the constitutive equation for the heat vector (in contra- and co-variant bases) for Oldroyd-B fluids. Fourier heat conduction law is generally used as the constitutive model for the heat vector for these fluids also.

## 7 Summary and conclusions

We have presented development of the rate constitutive theory for ordered thermoviscoelastic fluids in contra- and co-variant bases. The theory considers convected time derivatives of up to order ‘ $m$ ’ of the deviatoric Cauchy stress tensor and convected time derivatives of up to order ‘ $n$ ’ of the strain tensor in the chosen basis. The convected time derivative of order ‘ $m$ ’ of the deviatoric Cauchy stress tensor, the heat vector  $\bar{\mathbf{q}}$  and Helmholtz free energy density  $\bar{\Phi}$  are considered as dependent variables in the development of the rate constitutive theory. Based on the principle of equipresence, the argument tensors of these dependent variables are considered to be  $[\gamma^{(j)}]$ ;  $j = 1, 2, \dots, n$ ,  $[d\bar{\sigma}^{(k)}]$ ;  $k = 0, 1, \dots, m - 1$ , density  $\bar{\rho}$ , temperature  $\bar{\theta}$  and temperature gradient  $\bar{\mathbf{g}}$  in the contra-variant basis. In the case of co-variant basis,  $[\gamma^{(j)}]$  and  $[d\bar{\sigma}^{(k)}]$  are replaced by  $[\gamma_{(j)}]$  and  $[d\bar{\sigma}_{(k)}]$  while the other arguments remain the same. This rate constitutive theory defines an ordered thermoviscoelastic fluid of orders  $(m, n)$ .

Many remarks made in chapters 2 and 3, and papers by Surana et al. [14, 26] regarding the second law of thermodynamics, conditions resulting from it, decomposition of the total stress tensor in equilibrium and deviatoric stress tensors, determination of equilibrium stress for incompressible and compressible cases leading to mechanical and thermodynamic pressure remain the same here as well and hence are not repeated for the sake of brevity. As in references [14, 26], here also, the second law of thermodynamics does not provide a mechanism for determining the constitutive equations for the deviatoric stress tensor but only requires that the dissipation due to deviatoric stress be positive. The development of the rate constitutive theory presented in this chapter is based on the theory of generators and invariants. In this approach  $[d\bar{\sigma}^{(m)}]$  and  $\bar{\mathbf{q}}$  or  $[d\bar{\sigma}_{(m)}]$  and  $\bar{\mathbf{q}}$  are expressed as a linear combination of the combined generators of the argument tensors keeping in mind that  $[d\bar{\sigma}^{(m)}]$  and  $[d\bar{\sigma}_{(m)}]$  are symmetric tensors of rank two where as  $\bar{\mathbf{q}}$  is a tensor of rank one. Hence, the combined generators used in the linear combinations for  $[d\bar{\sigma}^{(m)}]$  or  $[d\bar{\sigma}_{(m)}]$  must also be symmetric tensors of rank two. Whereas the combined generators used to define  $\bar{\mathbf{q}}$  must be tensors of rank one. Additionally we must also adhere to minimal basis in these linear combinations. The coefficients in the linear combinations are functions of density  $\bar{\rho}$ , temperature  $\bar{\theta}$  and the combined invariants of the argument tensors of rank one and two and are determined by considering their Taylor series expansion about the reference configuration and limiting the expansion up to linear terms in the combined invariants and  $\bar{\theta}$ . We make the following specific remarks based on the work presented in this chapter.

1. The general theory of the rate constitutive equations for ordered thermoviscoelastic fluids of orders  $(m, n)$  is presented for compressible as well as incompressible thermoviscoelastic fluids.
2. The general theory of rate constitutive equations is specialized for  $m = 1$  and  $n = 1$ , i.e., thermoviscoelastic fluids of order one in deviatoric Cauchy stress and strain rates. In this case  $[d\bar{\sigma}^{(1)}]$  or  $[d\bar{\sigma}_{(1)}]$  contain  $[d\bar{\sigma}^{(0)}]$ ,  $[\gamma^{(1)}]$ ,  $\bar{\rho}$ ,  $\bar{\theta}$ ,  $\bar{\mathbf{g}}$  or  $[d\bar{\sigma}_{(0)}]$ ,  $[\gamma_{(1)}]$ ,  $\bar{\rho}$ ,  $\bar{\theta}$ ,  $\bar{\mathbf{g}}$  as argument tensors in contra- and co-variant bases. The same argument tensors also hold for the heat vector  $\bar{\mathbf{q}}$ .
3. The general theory is also specialized for  $m = 1$  and  $n = 2$ , i.e., thermoviscoelastic fluids of order one in deviatoric Cauchy stress rate but of order two in strain rate. In this case  $[d\bar{\sigma}^{(1)}]$  or  $[d\bar{\sigma}_{(1)}]$  contain  $[d\bar{\sigma}^{(0)}]$ ,  $[\gamma^{(1)}]$ ,  $[\gamma^{(2)}]$ ,  $\bar{\rho}$ ,  $\bar{\theta}$ ,  $\bar{\mathbf{g}}$  or  $[d\bar{\sigma}_{(0)}]$ ,  $[\gamma_{(1)}]$ ,  $[\gamma_{(2)}]$ ,  $\bar{\rho}$ ,  $\bar{\theta}$ ,  $\bar{\mathbf{g}}$  as argument tensors in contra- and co-variant bases. The same argument tensors also hold for the heat vector  $\bar{\mathbf{q}}$ .

4. The contra-variant basis yields upper convected ordered rate constitutive equations. Likewise, co-variant basis yields lower convected ordered rate constitutive equations. Surana et al. [28] have shown that only contra-variant basis is in accordance with the physics of deforming matter when the deformation is finite. As the deformation deviates from the infinitesimal assumption, the rate constitutive equations based on co-variant basis and others (such as Jaumann rate equations) become progressively spurious with progressively increasing deformation.
5. It is shown that Maxwell constitutive model and Giesekus constitutive model are a subset of ordered thermoviscoelastic fluids (incompressible) of orders  $m = 1$  and  $n = 1$ . Derivations presented in this chapter demonstrate many assumptions needed for the general case of  $m = 1, n = 1$  to derive these constitutive models. Maxwell model is a linear viscoelastic model whereas Giesekus constitutive model is a non-linear constitutive model.
6. It is also shown that Oldroyd-B constitutive model is a subset of the rate constitutive equations of orders  $m = 1$  and  $n = 2$ . The derivation presented in this chapter demonstrates many assumptions that must be employed for the general case of  $m = 1$  and  $n = 2$  to derive Oldroyd-B constitutive model. This constitutive model is referred to as quasi-linear constitutive model.
7. The Maxwell, Oldroyd-B and Giesekus constitutive models as used in polymer science have been derived using kinetic theory [5, 11]. The reference to the Maxwell model based on continuum mechanics can be found in [12, 13]. However, the derivations of Oldroyd-B and Giesekus constitutive models based on principles and axioms of continuum mechanics as presented in this chapter are the first appearance of this work in the published literature to our knowledge.
8. The derivations of Maxwell, Oldroyd-B and Giesekus constitutive models presented here are fundamental in understanding the assumptions employed in their derivations which eventually limit their range of applications. For example, all three constitutive models are only valid for non-finite deformation for which the distinction between co- and contra-variant bases is irrelevant. Giesekus model is superior in terms of more realistic  $[\bar{d}\bar{\sigma}^{(0)}]$  or  $[\bar{d}\bar{\sigma}_{(0)}]$  due to inclusion of  $[\bar{d}\bar{\sigma}^{(0)}]^2$  or  $[\bar{d}\bar{\sigma}_{(0)}]^2$ .
9. This chapter also presents the constitutive theory for  $\bar{\mathbf{q}}$  that contains same argument tensors as  $[\bar{d}\bar{\sigma}^{(m)}]$  or  $[\bar{d}\bar{\sigma}_{(m)}]$ . This is essential for consistency of the constitutive theory.
10. All developments consider the fluid to be compressible as well as incompressible in both contra- and co-variant bases.
11. We remark that decomposition of the Cauchy stress tensor into equilibrium stress and deviatoric Cauchy stress is necessitated by the second law of thermodynamics and it clearly shows that the development of rate constitutive theory must consider deviatoric Cauchy stress which is indeed the case for Maxwell and Oldroyd-B models used in polymer science community. However, in the case of Giesekus constitutive model as used presently in the polymer science community, the deviatoric Cauchy stress is further decomposed as follows (consider contra-variant basis)

$$[\bar{d}\bar{\sigma}^{(0)}] = [\bar{d}\bar{\sigma}^{(0)}]_s + [\bar{d}\bar{\sigma}^{(0)}]_p$$

where ‘s’ refers to solvent stress and ‘p’ refers to polymer stress consisting of viscous and elastic components.  $[\bar{d}\bar{\sigma}^{(0)}]_s$  is defined using Newton’s law of viscosity [5]. The rate constitutive equations used currently are defined using polymer stress  $[\bar{d}\bar{\sigma}^{(0)}]_p$ . We make the following remarks.

- (a) The development of the constitutive theory based on the second law of thermodynamics must consider  $[\bar{d}\bar{\sigma}^{(0)}]$  as a dependent variable in the constitutive theory and not the polymer stress.
- (b) Within the continuum mechanics framework, there is no basis for the decomposition shown above as well as no basis for expressing  $[\bar{d}\bar{\sigma}^{(0)}]_s$  using Newton’s law of viscosity as done presently. Instead this must be derivable within the constitutive theory framework.
- (c) Use of  $[\bar{d}\bar{\sigma}^{(0)}]_p$  in the constitutive theory may be justifiable based on kinetic theory or other physical arguments but there is no basis for using it as a dependent variable in the constitutive theory within the framework of continuum mechanics in the development of the rate constitutive equations.

- (d) The rate constitutive theory presented in this chapter always considers deviatoric Cauchy stress as a dependent variable in the development of the theory and not its further decomposition as used currently. It is a simple and straight forward matter to see that if we consider rate constitutive equations in deviatoric Cauchy stress as presented here and if we substitutive the decomposition shown above, then  $[_d\bar{\sigma}^{(0)}]_s$  based on Newton's law of viscosity is a necessary assumption to eliminate  $[_d\bar{\sigma}^{(0)}]_s$  as dependent variables in the constitutive theory.
12. In polymer science, it is argued [29, 30] that decomposition of the deviatoric Cauchy stress in terms of viscous (both solvent and polymer) and elastic components and then expressing viscous stress using Newton's law of viscosity and thus obtaining constitutive equations in terms of elastic stress is meritorious (computationally). This approach has two fundamental problems if viewed based on the principles and axioms of continuum mechanics for constitutive theory. First, the deviatoric Cauchy stress must be a dependent variable in the constitutive theory and not the elastic stress. This argument questions the decomposition. Secondly, use of Newton's law of viscosity must be derivable as opposed to simply using it as a constitutive theory for the viscous stress tensor.
  13. Since the constitutive theory presented here is based on combined generators and invariants of the argument tensors of the dependent variable, strictly speaking it lacks thermodynamic basis (as these are not derived using entropy inequality). However, the theory does have continuum mechanics foundation and it does satisfy the conditions resulting from entropy inequality.

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## Chapter 5

# The Rate Constitutive Equations and their Validity for Progressively Increasing Deformation

The rate constitutive equations based on upper convected, lower convected, Jaumann, Truesdell and Green-Naghdi stress rates etc. [1–10] have been used for the solid matter and polymeric liquids when the mathematical models are derived employing conservation laws in Eulerian description. The rate constitutive equations provide relationship between convected time derivatives of the stress tensor and the convected time derivatives of strain tensor through the constitution of the matter. It is well known that if one assume constant properties of the matter, then the use various rate constitutive equations yield different responses [9] when the strains and strain rates are not infinitesimal (finite deformation) even though the rate constitutive equations are objective or frame invariant. This has been rationalized by the argument that in order for the different rate constitutive equations to produce the same response, the material tensor must be different for each case[9]. Our point of view is rather pragmatic in the sense that if all rate constitutive models describe the behavior of the same matter in which material constants do not change during deformation, then surely there must be some inherent assumptions in their derivations that are responsible for this anomaly.

The co-variant and contra-variant convected bases in the current configuration of the deforming matter provide two possible alternate means of defining the convected time derivatives of the contra- and co- variant Cauchy stress tensors as well as the strain tensors. Relationship between the convected time derivatives of the stress tensor, material tensor and convected time derivative of the strain tensor result in the rate constitutive equations. Thus there are at least two obvious approaches for deriving rate constitutive equations : one based on co-variant description referred to as lower convected rate constitutive equations and the other based on contra-variant description referred to as upper convected rate constitutive equations. It can be shown that the other rate constitutive equations available (in the literature) can also be derived using these two basic descriptions by modifications that are either justified based on the physics of the deforming matter or mathematical manipulations. When the strains and the strain rates are small (closer to infinitesimal assumption), there is isomorphism (or equivalence) between the co-variant and contra-variant descriptions, hence in this case the two descriptions will yield identical results even though the explicit forms of the rate equation expressions in the two descriptions are different. It is shown that when the strains and the strain rates are finite (finite deformation), the isomorphism or equivalence between the two descriptions is lost. This chapter demonstrates that with progressively increasing deformation leading to finite deformation only the contra-variant description has physical basis, hence the rate constitutive equations derived using contra-variant description remain valid whereas all others become spurious. Detailed mathematical development of the rate constitutive equations based on co-variant, contra-variant descriptions and others based on these two bases are presented to illustrate their validity and limitations. Numerical examples are also presented using Giesekus constitutive model for dense polymeric liquids (polymer melts) to demonstrate the validity of contra-variant basis and the failures of co-variant and others commonly used in the literature.

The research work presented in this chapter has been submitted for journal publication and is in press [11].

# 1 Introduction and approach

The development of the mathematical models for deforming matter based on conservation laws in Eulerian description necessitates the use of velocities as dependent variables particularly for liquids and gases. Closure to the resulting partial differential equations is provided by the constitutive equations and the equation(s) of state (if the matter is compressible). The constitutive equations describing constitution of the matter require: (i) A relationship between heat flux, temperature gradients and conductivity of the matter. The Fourier heat conduction law suffices for this purpose. This presents no difficulty in the Eulerian description. (ii) A relationship that describes how the deformation of the matter and its properties are related to the internal stress field developed in the deforming matter. In this chapter the constitutive equations refer to this aspect of the constitution of the matter and are used in this context henceforth. Use of velocities as dependent variables in the conservation laws in Eulerian description necessitates that the constitutive equations for the deforming matter must utilize velocities as well (as opposed to displacements). The convected coordinate system synchronous with the deformation is ideal due to the fact that curvilinear axes in this coordinate system are the material lines in the current configuration. The frame invariant requirement of the constitutive equations precludes all other options except time derivatives of the appropriate stress and strain measures in the convected coordinate system. The relationships between the convected time derivatives of the stress and strain tensors and the material tensor are referred to as rate constitutive equations. The necessity of using these rate constitutive equations naturally arises when the mathematical models for the deforming matter are developed using Eulerian description. In case of solid matter, upper convected, lower convected, Jaumann, Truesdell, Green-Naghdi etc. stress rates are commonly used in the rate constitutive equations. In case of polymer flows the constitutive models such as Maxwell, Oldroyd-B, Giesekus etc. are all rate constitutive models that may also be based on the same stress rates as used for solid matter. The choice of appropriate and physical conjugate pairs of stress and strain measures and their convected time derivatives are critical in order for the rate constitutive mathematical models to be meaningful.

The final forms of the rate constitutive equations such as upper convected, lower convected, Jaumann, Truesdell, Green-Naghdi etc. and the details pertaining to these for solid matter can be found in references [1–10]. When the deformation is infinitesimal and hence small strain and small strain rates, all commonly used rate constitutive equations yield almost the same behavior. In case of progressively increasing deformation approaching finite deformation and hence finite strain and finite strain rates this is not the case [9]. Thus, it is natural to ask which rate equations are closer to the real physics of the deforming matter. In published works such as reference [9], it is stated that in order for the different rate equations to produce same material response (when the strain or strain rates are finite i.e. finite deformation) for a given matter, the material tensor must be different in each case. Perhaps so, but our view point is that for a matter with constant properties, the material tensor is constant, hence the anomalies observed in the material response by the use of different rate equations in the mathematical models must surely be due to some more fundamental reasons and/or assumption employed in their derivations. In reference [12], one dimensional and two dimensional wave propagation studies in linear elastic medium were presented to demonstrate that with progressively increasing strain only upper convected rate constitutive equation produces physically meaningful results, but no theoretical development or any other explanation was provided for the observed behaviors. In this chapter we consider rate constitutive equations for solid, Newtonian fluids as well as polymeric liquids. The work presented in this chapter discusses fundamental approach for deriving various rate constitutive equations, points out the assumption employed, explains the reasons for physical or anomalous behaviors and presents numerical studies as illustrations.

## 2 Notations; coordinate system; bases; measures of strains, stresses, their convected time derivatives and derivations of the rate constitutive equations

Consider undeformed matter in the reference configuration at time  $t_0$  (could be assumed zero) shown in Figure 5.1(a). The reference configuration which could be different than the configuration of the matter at time  $t_0$  but assumed same for simplicity of derivations. Consider a volume of matter  $V$  with closed boundary  $\partial V$  and an elementary tetrahedron  $oABC$  with its face  $ABC$  coincident with the boundary  $\partial V$ . Let  $ox_1x_2x_3$  be an

orthogonal Cartesian coordinate system located at point  $o$  (in the matter or outside the matter) . Then each material particle can be assigned a unique label  $(x_1, x_2, x_3)$ , its coordinates in  $ox_1x_2x_3$  frame and hence uniquely identified. Assume that the matter is homogeneous and isotropic. Let  $ox_1, ox_2, ox_3$  parallel to  $x_1, x_2, x_3$  axes of the  $ox_1x_2x_3$  frame be the material lines coincident and co-linear with edges of the tetrahedron  $oABC$  (Figure 5.1(a) and (b)). Upon deformation the material particles assume position in the current configuration (Figure 5.2) at time  $t$ . The volume  $V$  deforms into  $\bar{V}(t)$  with its boundary  $\partial\bar{V}(t)$ . The elementary tetrahedron  $oABC$  deforms into  $\bar{o}\bar{A}\bar{B}\bar{C}$  with its deformed edges  $\bar{o}\bar{A}, \bar{o}\bar{B}$  and  $\bar{o}\bar{C}$  coincident with the curvilinear axes  $\bar{o}\bar{x}_1, \bar{o}\bar{x}_2$  and  $\bar{o}\bar{x}_3$ . The coordinate system  $\bar{o}\bar{x}_1\bar{x}_2\bar{x}_3$  is called convected coordinate system. If  $\bar{P}$  is the resultant force exerted on the face  $\bar{A}\bar{B}\bar{C}$  of the deformed tetrahedron by the volume of the matter surrounding boundary  $\partial\bar{V}(t)$  and if  $\bar{n}$  is the unit exterior normal to the face  $\bar{A}\bar{B}\bar{C}$  of the deformed tetrahedron, then by considering equilibrium of the deformed tetrahedron, we could develop various measures of the stresses acting on the deformed faces  $\bar{o}\bar{A}\bar{B}, \bar{o}\bar{B}\bar{C}$  and  $\bar{o}\bar{C}\bar{A}$  of the tetrahedron  $\bar{o}\bar{A}\bar{B}\bar{C}$ . Likewise conjugate strain measures can be derived as well. The convected coordinate system  $\bar{o}\bar{x}_1\bar{x}_2\bar{x}_3$  is crucial in developing constitutive equations due to the fact that this coordinate system defines deformed material lines in the current configuration.

Let the vectors  $\tilde{g}_1, \tilde{g}_2$  and  $\tilde{g}_3$  be tangent to the  $\bar{o}\bar{x}_1, \bar{o}\bar{x}_2$  and  $\bar{o}\bar{x}_3$  at material point  $\bar{o}$ . The vectors  $\tilde{g}_i$  (not normalized) are called co-variant base or basis vectors. The basis vectors  $\tilde{g}_i$  define a non-orthogonal basis and form the faces of the deformed tetrahedron.

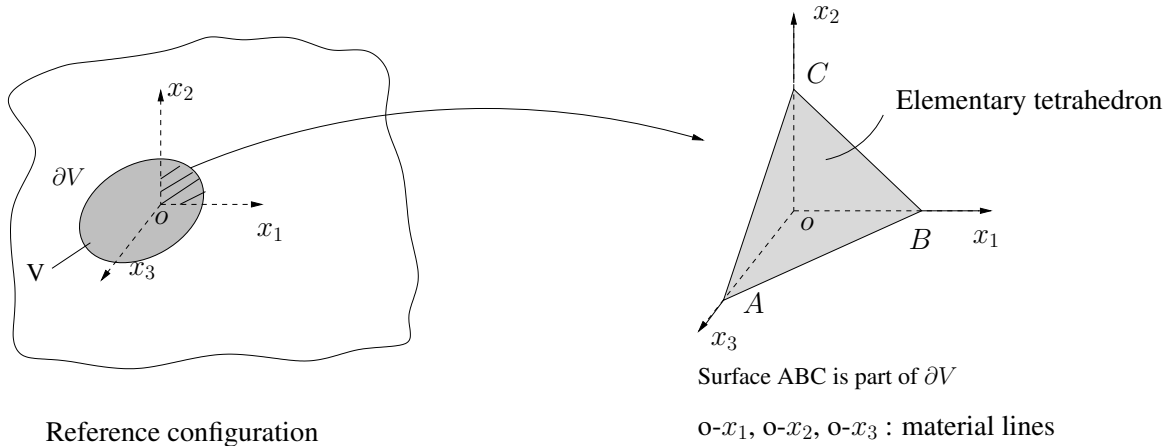


Figure 5.1: Elementary tetrahedron in the reference configuration

We can also introduce another set of base vectors called reciprocal base vectors  $\tilde{g}^i$  using

$$\tilde{g}^1 = (\tilde{g}_2 \times \tilde{g}_3) \quad ; \quad \tilde{g}^2 = (\tilde{g}_3 \times \tilde{g}_1) \quad ; \quad \tilde{g}^3 = (\tilde{g}_1 \times \tilde{g}_2) \quad (2.1)$$

The base vectors  $\tilde{g}^i$  are called contra-variant base vectors. We note that  $\tilde{g}^1$  is normal to the face of the  $\bar{o}\bar{A}\bar{C}$  formed by the co-variant base vectors  $\tilde{g}_2$  and  $\tilde{g}_3$ . Likewise  $\tilde{g}^2$  and  $\tilde{g}^3$  are normal to the faces  $\bar{o}\bar{A}\bar{B}$  and  $\bar{o}\bar{B}\bar{C}$  of the deformed tetrahedron  $\bar{o}\bar{A}\bar{B}\bar{C}$ . The volume of the deformed parallelepiped formed by the vectors  $\tilde{g}_i$  is given by  $\bar{V} = \tilde{g}_1 \cdot (\tilde{g}_2 \times \tilde{g}_3)$ . Using (2.1) it is straight forward to see that the following holds:

$$\tilde{g}^i \cdot \tilde{g}_j = \tilde{g}_i \cdot \tilde{g}^j = \bar{V} \delta_{ij} \quad (2.2)$$

where  $\delta_{ij}$  is Kronecker delta.

If we designate the coordinates of the material points in the current configuration by  $\bar{x}_1, \bar{x}_2, \bar{x}_3$ , measured with respect to  $ox_1x_2x_3$  frame, then a material point in the current configuration can be identified by

$$\bar{x}_i = \bar{x}_i(x_1, x_2, x_3, t) \quad (2.3)$$

Inverse of (2.3) gives

$$x_i = x_i(\bar{x}_1, \bar{x}_2, \bar{x}_3, t) \quad (2.4)$$

using (2.3) and (2.4) it is possible to precisely define co-variant and contra-variant base vectors. Consider material particles  $P(x_i)$  and  $Q(x_i + dx_i)$  in the reference configuration . Let  $\bar{P}, \bar{Q}$  be their locations in the

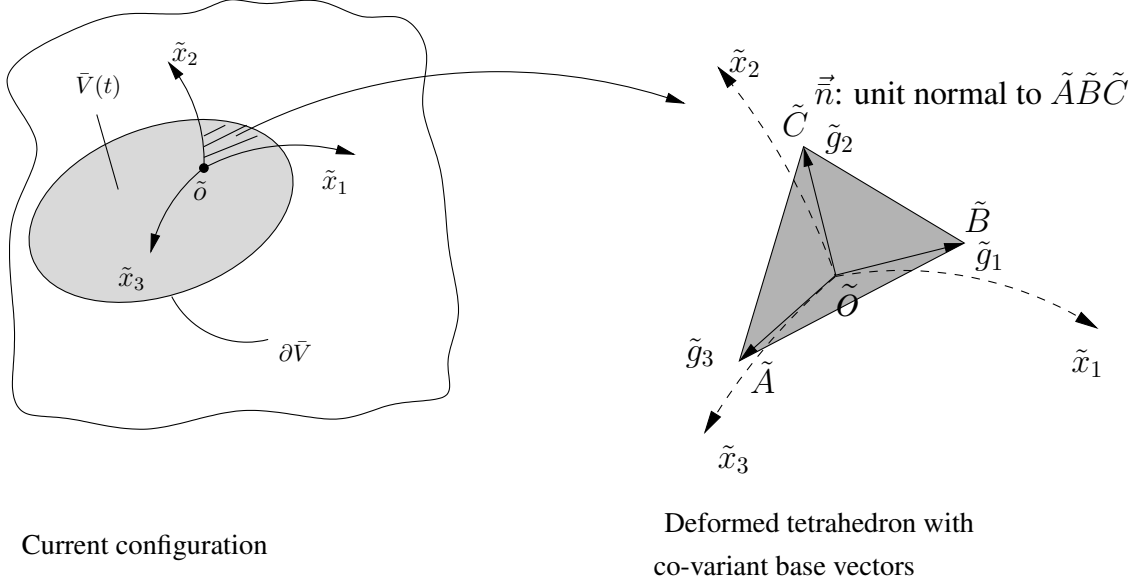


Figure 5.2: Deformed elementary tetrahedron in the current configuration

current configuration. Thus vector  $\overrightarrow{PQ}$  in the reference configuration is deformed into  $\overrightarrow{PQ}$  in the current configuration. Let the motion of the matter be given by (2.3) in which  $\bar{x}_i(x_1, x_2, x_3, t)$  are continuous and differentiable functions of their arguments. Then

$$\overrightarrow{PQ} = (\bar{x}_i(x_1 + dx_1, x_2 + dx_2, x_3 + dx_3, t) - \bar{x}_i(x_1, x_2, x_3, t))e_i \quad (2.5)$$

where  $e_i$  are unit vectors along  $ox_i$  axes.

Using Taylor series expansion of the first term at  $P(x_i)$  and retaining up to the second order terms in  $dx_i$

$$\overrightarrow{PQ} = (\bar{x}_i(x_1, x_2, x_3, t) + \frac{\partial \bar{x}_i}{\partial x_j} dx_j + \frac{1}{2} \frac{\partial^2 \bar{x}_i}{\partial x_j \partial x_k} dx_j dx_k + O(|dx|^3) - \bar{x}_i(x_1, x_2, x_3, t))e_i \quad (2.6)$$

Neglecting  $O(|dx|^3)$  in (2.6), we obtain the following for  $\overrightarrow{PQ}$

$$\overrightarrow{PQ} = \frac{\partial \bar{x}_i}{\partial x_j} dx_j e_i + \frac{1}{2} \frac{\partial^2 \bar{x}_i}{\partial x_j \partial x_k} dx_j dx_k e_i \quad (2.7)$$

where

$$\overrightarrow{PQ} = [d\bar{x}_1, d\bar{x}_2, d\bar{x}_3]^t \quad (2.8)$$

(2.7) is a fundamental relation that express how the deformed lengths  $d\bar{x}_i$  are related to undeformed length with the assumption that the infinitesimals of order three and higher in lengths are negligible. Using (2.4) and following the procedure used in deriving (2.7), we can also write

$$\overrightarrow{PQ} = \frac{\partial x_i}{\partial \bar{x}_j} d\bar{x}_j e_i + \frac{1}{2} \frac{\partial^2 x_i}{\partial \bar{x}_j \partial \bar{x}_k} d\bar{x}_j d\bar{x}_k e_i \quad (2.9)$$

where  $\overrightarrow{PQ} = [dx_1, dx_2, dx_3]^t$ . In (2.9) also, the infinitesimals of order three and higher in lengths have been neglected. When the deformation is such that infinitesimals of order two of lengths can be neglected, expression (2.7) and (2.9) reduce to

$$\overrightarrow{PQ} = \frac{\partial \bar{x}_i}{\partial x_j} dx_j e_i \quad (2.10)$$

$$\overrightarrow{PQ} = \frac{\partial x_i}{\partial \bar{x}_j} d\bar{x}_j e_i \quad (2.11)$$

or in the matrix form

$$\{d\bar{x}\} = [J]\{dx\} \quad (2.12)$$

$$\{dx\} = [\bar{J}]\{d\bar{x}\} \quad (2.13)$$

(2.12) is the co-variant transformation where as (2.13) is the contra-variant transformation. Thus  $[J]$  and  $[\bar{J}]$  contain information regarding the co-variant and the contra-variant bases. From (2.12) and (2.13) we note that at material point  $\bar{P}$

$$[J] = [\bar{J}]^{-1} \quad ; \quad [\bar{J}] = [J]^{-1} \quad \text{and} \quad [J][\bar{J}] = [\bar{J}][J] = [I] \quad (2.14)$$

$[J]$  is referred to as Jacobian of deformation.

It is significant note that columns of  $[J]$  are co-variant base vectors whereas the contra-variant base vectors are rows of  $[\bar{J}]$ . This distinction between  $[J]$  and  $[\bar{J}]$  is extremely significant when using  $[J]$  and  $[\bar{J}]$  to define measures of finite strains. A straight forward derivation of Green's strain and Almansi strain based on undeformed and deformed line segments  $ds$  and  $d\bar{s}$  in reference and current configurations using  $[J]$  and  $[\bar{J}]$  yield the following for Green's strain  $[\varepsilon]$  (co-variant measure) and Almansi strain  $[\bar{\varepsilon}]$  (contra-variant measure).

$$[\varepsilon] = \frac{1}{2}([J]^t[J] - [I]) \quad (2.15)$$

in which  $[\varepsilon]$  contains Cartesian components based on the fact that columns of  $[J]$  are co-variant base vectors. The components of  $[\varepsilon]$  correspond to the correct dyads in the Cartesian frame (say  $x$ -frame).

For Almansi strain we have

$$[\bar{\varepsilon}] = \frac{1}{2}([I] - [\bar{J}]^t[\bar{J}]) \quad (2.16)$$

in which  $[\bar{\varepsilon}]$  also contains Cartesian components but based on the fact that contra-variant base vectors are rows of  $[\bar{J}]$  and not the columns. Thus the components of  $[\bar{\varepsilon}]$  do not correspond to the correct dyads in the Cartesian frame. To correct this situation we must use a different form of  $[\bar{J}]$  in the definition of  $[\bar{\varepsilon}]$  in which the columns are the contra-variant base vector. This of course can be done by using transpose of  $[\bar{J}]$ . Thus in (2.16)  $[\bar{J}]$  must be replaced with  $[\bar{J}]^t$  which yields the following definition of Almansi strain

$$[\bar{\varepsilon}] = \frac{1}{2}([I] - [\bar{J}][\bar{J}]^t) \quad (2.17)$$

The components of  $[\varepsilon]$  in (2.16) and those of  $[\bar{\varepsilon}]$  in (2.17) have the same and correct dyads. In deriving convected rates we must ensure that definitions of  $[\varepsilon]$  and  $[\bar{\varepsilon}]$  in (2.15) and (2.17) are used instead of  $[\bar{\varepsilon}]$  defined by (2.16).

We note the relation (2.12) and (2.13) have assumption that infinitesimals of the lengths of order two can be neglected but, (2.14) hold regardless of the magnitude of deformation and hence can be used wherever and whenever in the subsequent derivations. A volume  $dx_1 dx_2 dx_3$  at material point  $P$  in the reference or undeformed configuration deforms into a parallelepiped. Co-variant base vectors is a natural way to identify this volume. The contra-variant base vectors  $\bar{g}^i$  are normal to the faces of the deformed volume i.e. parallelepiped or the tetrahedron. The definition of strains, stresses and their time derivatives in these two bases are of interest. If we choose directions  $ox_1$ ,  $ox_2$  and  $ox_3$  with base vectors  $e_1$ ,  $e_2$  and  $e_3$ , then we can define a stress tensor  $[\sigma]$  as follows

$$[\sigma] = e_i e_j \sigma_{ij} \quad (2.18)$$

On the other hand, a more natural way to define stresses is to use the current configuration (Figure 5.2) and to consider the deformed volume, that is the elementary tetrahedron with direction  $\bar{g}^i$  normal to the faces of the deformed tetrahedron. On each face we have a stress in the direction of the normal (normal stress) and the other two (shear stresses) in the remaining two directions. This description of the stress is contra-variant description or contra-variant Cauchy stress tensor  $[\bar{\sigma}^{(0)}]$ . Using the base vectors  $\bar{g}^i$ , we could easily obtain its corresponding components in  $ox_1$ ,  $ox_2$  and  $ox_3$  directions (Cartesian components). Since the directions  $\bar{g}^i$  are obtained using (2.1), it is natural to expect appearance of the co-variant basis (equation (2.27)) in defining the Cartesian components of  $[\bar{\sigma}^{(0)}]$ . The contra-variant stress definition corresponds to faces of the actual deformed tetrahedron and hence, has physical basis.

Another possible way to define the stresses in the current configuration is to consider co-variant direction  $\tilde{g}_i$ . That is we consider a stress component in one of the  $\tilde{g}_i$  directions (normal stress) and the other two

corresponding to the remaining two  $\tilde{\mathbf{g}}_i$  directions. In terms of physics, we are essentially considering a new tetrahedron that is obtained by appropriate distortion (shown later) of the tetrahedron of Figure 5.2 such that  $\tilde{\mathbf{g}}_i$  directions are perpendicular to the faces of this new tetrahedron. The stresses defined using  $\tilde{\mathbf{g}}_i$  directions that correspond the faces of a new distorted deformed tetrahedron obtained from that of Figure 5.2 are called co-variant Cauchy stress tensor  $[\bar{\sigma}_{(0)}]$ . Using the co-variant base vectors  $\tilde{\mathbf{g}}_i$ , we could obtain its components in the  $ox_1x_2x_3$  coordinate system. The fact that co-variant description of the stress requires further distortion of the actual deformed tetrahedron is significant to note. First, we note that contra-variant stress description utilizes actual deformed volume (Figure 5.2) and hence has physical basis. Description of the co-variant stress tensor using the faces of a new distorted tetrahedron in which  $\tilde{\mathbf{g}}_i$  are normal to its faces has no physical basis. Secondly, when the strains are infinitesimal, the two stress descriptions can be shown to be almost identical which is not surprising because in this case the distortion of the tetrahedron of Figure 5.2 is negligible hence,  $\tilde{\mathbf{g}}_i$  and  $\tilde{\mathbf{g}}^i$  directions coincide. For such cases the rate constitutive equations can be derived using either one of the stress description without detriment. When the deformation is finite in which case the strains are not infinitesimal, the distortion of the tetrahedron of Figure 5.2 required to obtain co-variant description can not be neglected and hence  $\tilde{\mathbf{g}}_i$  and  $\tilde{\mathbf{g}}^i$  directions no longer coincide. In such cases only contra-variant stress description is physical and valid. Larger the deformation, larger are the strains and hence more is the deviation in the directions  $\tilde{\mathbf{g}}_i$  and  $\tilde{\mathbf{g}}^i$  and therefore more spuriousness can be expected due to the use of rate constitutive equations based on co-variant description and others that are not purely based on contra-variant description (see numerical studies).

## 2.1 Contra-variant and co-variant stress tensors

First we consider the contra-variant stress tensor and its Cartesian components. The Cartesian components of the contra-variant stress tensor can be derived using either of the two approaches: 1) Consideration of deformed and undeformed areas, normals to them, the resultant forces acting on them and a correspondence rule. 2) Using  $[\bar{\sigma}^{(0)}]$  and the contra-variant base vectors  $\tilde{\mathbf{g}}^i$ . In the derivation presented in the following, we consider the first approach for deriving Cartesian components of the contra-variant stress tensor. The derivation for co-variant case follows parallel procedure. Consider Figure 5.3. Let  $dA_n$  be a typical undeformed area with normal  $\vec{n}$ , which in the current configuration becomes  $d\tilde{A}_n$  with normal  $\vec{\tilde{n}}$ . Let  $\{dF\}$  be the resultant force acting on this area  $dA_n$ . Let  $\{d\tilde{F}\}$  be the resultant force acting on area  $d\tilde{A}_n$  producing stresses  $[\sigma]$ , the Cartesian components of  $[\bar{\sigma}^{(0)}]$ , then, we assume that  $\{dF\}$  acting on  $dA_n$  and  $\{d\tilde{F}\}$  acting on  $d\tilde{A}_n$  are related through the Jacobian of deformation  $[J]$  (correspondence rule)

$$\{d\tilde{F}\} = [J]\{dF\} \quad (2.19)$$

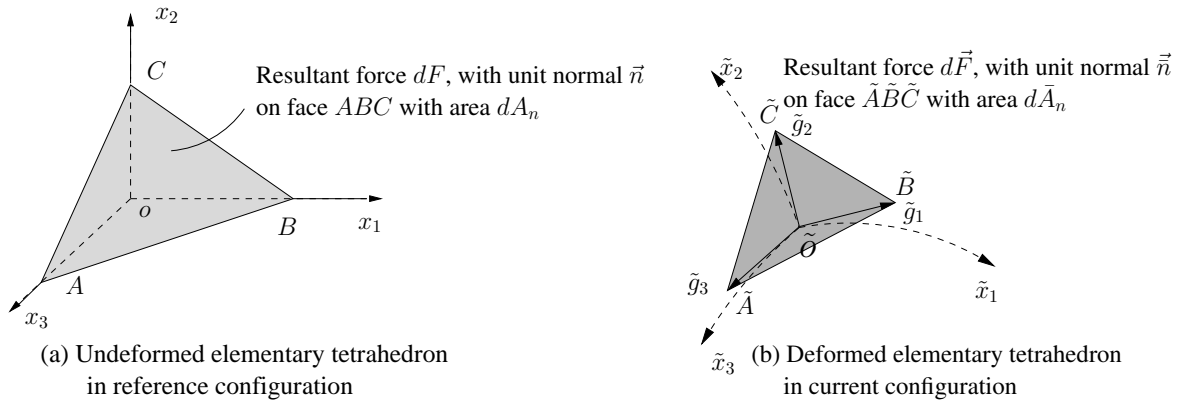


Figure 5.3: Undeformed and deformed elementary tetrahedron

Thus application of stress  $[\sigma]$  to area  $dA_n$  in the undeformed state yields the force vector  $\{dF\}$

$$\{dF\} = dA_n[\sigma]^t\{n\} = [\sigma]^t\{dA\} \quad (2.20)$$

$$\text{also } \{d\bar{F}\} = d\bar{A}_n[\bar{\sigma}^{(0)}]^t\{\bar{n}\} = [\bar{\sigma}^{(0)}]^t\{d\bar{A}\} \quad (2.21)$$

$$\text{But } \{d\bar{A}\} = |J|[J^t]^{-1}\{dA\} \quad (2.22)$$

$$\{d\bar{F}\} = |J|[\bar{\sigma}^{(0)}]^t[J^t]^{-1}\{dA\} \quad (2.23)$$

But  $\{d\bar{F}\}$  can also be obtained using (2.19) and (2.20)

$$\{d\bar{F}\} = [J][\sigma]^t\{dA\} \quad (2.24)$$

Equating (2.23) and (2.24) gives

$$[J][\sigma]^t\{dA\} = |J|[\bar{\sigma}^{(0)}]^t[J^t]^{-1}\{dA\} \quad (2.25)$$

But  $\{dA\}$  is arbitrary hence

$$[J][\sigma]^t = |J|[\bar{\sigma}^{(0)}]^t[J^t]^{-1} \quad (2.26)$$

$$\text{or } [\sigma]^t = |J|[J]^{-1}[\bar{\sigma}^{(0)}]^t[J^t]^{-1} \quad (2.27)$$

$$[\sigma]^t = |J|[\bar{J}][\bar{\sigma}^{(0)}]^t[\bar{J}]^t \quad \text{or} \quad [\sigma] = |J|[\bar{J}][\bar{\sigma}^{(0)}][\bar{J}]^t \quad (2.28)$$

i.e.  $[\sigma]$ , the Cartesian components of  $[\bar{\sigma}^{(0)}]$ , the contra-variant (Cauchy) stress tensor is also referred to as second Piolla-Kirchhoff stress tensor and is obviously symmetric. If the matter is incompressible then,  $|J| = 1$  and (2.28) becomes

$$[\sigma] = [\bar{J}][\bar{\sigma}^{(0)}][\bar{J}]^t = [\sigma^{[0]}] \quad (\text{Def.}) \quad (2.29)$$

The same results can be derived using the second approach. Following similar procedure or using the second approach mentioned earlier, we can show that the Cartesian components  $[\sigma_{[0]}]$  of the co-variant Cauchy stress tensor  $[\bar{\sigma}_{(0)}]$  are given by (for incompressible matter in which case  $|J| = 1$ )

$$[\sigma] = [J]^t[\bar{\sigma}_{(0)}][J] = [\sigma_{[0]}] \quad (\text{Def.}) \quad (2.30)$$

## 2.2 Convected time derivatives of the stress tensors

We note that  $[\bar{\sigma}^{(0)}]$  and  $[\bar{\sigma}_{(0)}]$  are stress tensor fields in spatial representation corresponding to convective (or convected) coordinate systems with contra- and co-variant components. In this section we present derivations of convected time derivatives of the tensors  $[\bar{\sigma}^{(0)}]$  and  $[\bar{\sigma}_{(0)}]$ . These will subsequently be used in the development of the rate constitutive equations. First we note a few useful relations. One could show that [10, 13]

$$\frac{D}{Dt}[J] = [L][J] \quad (2.31)$$

$$\text{where } [L] = \frac{\partial v_i}{\partial \bar{x}_j} \mathbf{e}_i \mathbf{e}_j \quad (2.32)$$

The material derivative of  $[\bar{J}]$  i.e.  $\frac{D}{Dt}[\bar{J}]$  can be obtained using the identity

$$[J][\bar{J}] = [I] \quad (2.33)$$

Taking material derivative of (2.33) (Product rule holds)

$$\frac{D}{Dt}([J][\bar{J}]) + [J]\frac{D}{Dt}[\bar{J}] = 0 \quad (2.34)$$

$$\text{or } \frac{D}{Dt}[\bar{J}] = -[J]^{-1}\frac{D}{Dt}([J])[\bar{J}] \quad (2.35)$$

Substituting from (2.31) into (2.35)

$$\frac{D}{Dt}[\bar{J}] = -[J]^{-1}[L][J][\bar{J}] \quad (2.36)$$

$$\frac{D}{Dt}[\bar{J}] = -[\bar{J}][L] \quad (2.37)$$

Equations (2.31) and (2.37) are the key expressions that are used in deriving convected time derivatives of tensors  $[\bar{\sigma}^{(0)}]$  and  $[\bar{\sigma}_{(0)}]$ .

Consider material derivative of  $[\sigma^{[0]}]$  given by (2.29)

$$\frac{D}{Dt}[\sigma^{[0]}] = \frac{D}{Dt}([\bar{J}][\bar{\sigma}^{(0)}][\bar{J}]^t) \quad (2.38)$$

$$\text{or } \frac{D}{Dt}[\sigma^{[0]}] = [\bar{J}] \frac{D}{Dt}([\bar{\sigma}^{(0)}])[\bar{J}]^t + \frac{D}{Dt}([\bar{J}])[\bar{\sigma}^{(0)}][\bar{J}]^t + [\bar{J}][\bar{\sigma}^{(0)}] \frac{D}{Dt}[\bar{J}]^t \quad (2.39)$$

Substituting from (2.37) into (2.39), regrouping and factoring yields

$$\frac{D}{Dt}[\sigma^{[0]}] = [\bar{J}] \left( \frac{D}{Dt}[\bar{\sigma}^{(0)}] - [L][\bar{\sigma}^{(0)}] - [\bar{\sigma}^{(0)}][L]^t \right) [\bar{J}]^t \quad (2.40)$$

Let us define

$$[\bar{\sigma}^{(1)}] = \frac{D}{Dt}[\bar{\sigma}^{(0)}] - [L][\bar{\sigma}^{(0)}] - [\bar{\sigma}^{(0)}][L]^t \quad (\text{Def.}) \quad (2.41)$$

Then if we denote

$$\frac{D}{Dt}[\sigma^{[0]}] = [\sigma^{[1]}] \quad (\text{Def.}) \quad (2.42)$$

We obtain the following from (2.40)

$$[\sigma^{[1]}] = [\bar{J}][\bar{\sigma}^{(1)}][\bar{J}]^t \quad (2.43)$$

$[\sigma^{(1)}]$  is the first convected time derivative of the contra-variant Cauchy stress tensor  $[\sigma^{(0)}]$  and hence generally referred to as contra-variant first convected time derivative or upper convected time derivative (of the contra-variant Cauchy stress tensor is implied). It is straight forward to show that one could also obtain the higher order convected time derivatives of the tensor  $[\sigma^{(0)}]$ . For example

$$[\sigma^{[2]}] = \frac{D}{Dt}[\sigma^{[1]}] = [\bar{J}][\bar{\sigma}^{(2)}][\bar{J}]^t \quad (2.44)$$

$$\text{where } [\bar{\sigma}^{(2)}] = \frac{D}{Dt}[\bar{\sigma}^{(1)}] - [L][\bar{\sigma}^{(1)}] - [\bar{\sigma}^{(1)}][L]^t \quad (2.45)$$

where  $[\bar{\sigma}^{(2)}]$  is the second convected time derivative of the contra-variant Cauchy stress tensor  $[\bar{\sigma}^{(0)}]$ , and so on.

The first upper convected time derivative is generally denoted by  $[\bar{\sigma}]$  and hence

$$[\bar{\sigma}] = [\bar{\sigma}^{(1)}] \quad (2.46)$$

Next we consider material derivative of the Cartesian components of the co-variant Cauchy stress tensor  $[\sigma_{[0]}]$  given by (2.30)

$$\frac{D}{Dt}[\sigma_{[0]}] = \frac{D}{Dt}([J]^t[\bar{\sigma}_{(0)}][J]) \quad (2.47)$$

$$\text{or } \frac{D}{Dt}[\sigma_{[0]}] = [J]^t \frac{D}{Dt}([\bar{\sigma}_{(0)}])[J] + \frac{D}{Dt}([J]^t)[\bar{\sigma}_{(0)}][J] + [J]^t[\bar{\sigma}_{(0)}] \frac{D}{Dt}[J] \quad (2.48)$$

Substituting from (2.31) into (2.48), regrouping and factoring gives

$$\frac{D}{Dt}[\sigma_{[0]}] = [J]^t \left( \frac{D}{Dt}[\bar{\sigma}_{(0)}] + [L]^t[\bar{\sigma}_{(0)}] + [\bar{\sigma}_{(0)}][L] \right) [J] \quad (2.49)$$

Let us define

$$[\bar{\sigma}_{(1)}] = \frac{D}{Dt}[\bar{\sigma}_{(0)}] + [L]^t[\bar{\sigma}_{(0)}] + [\bar{\sigma}_{(0)}][L] \quad (\text{Def.}) \quad (2.50)$$

Then if we denote

$$\frac{D}{Dt}[\sigma_{[0]}] = [\sigma_{[1]}] \quad (\text{Def.}) \quad (2.51)$$

We obtain the following from (2.49)

$$[\sigma_{[1]}] = [J]^t [\bar{\sigma}_{(1)}] [J] \quad (2.52)$$

$[\bar{\sigma}_{(1)}]$  is the first convected time derivative of the co-variant Cauchy stress tensor  $[\bar{\sigma}_{(0)}]$  and hence generally referred to as co-variant first convected time derivative or lower convected time derivative (of the co-variant Cauchy stress tensor is implied). In this case also, one could show that higher order convected time derivatives of  $[\bar{\sigma}_{(0)}]$  can be easily obtained, for example

$$[\sigma_{[2]}] = \frac{D}{Dt} [\sigma_{[1]}] = [J]^t [\bar{\sigma}_{(2)}] [J] \quad (2.53)$$

$$\text{where } [\bar{\sigma}_{(2)}] = \frac{D}{Dt} [\bar{\sigma}_{(1)}] + [L]^t [\bar{\sigma}_{(1)}] + [\bar{\sigma}_{(1)}] [L] \quad (2.54)$$

where  $[\bar{\sigma}_{(2)}]$  is the second convected time derivative of the co-variant Cauchy stress tensor  $[\bar{\sigma}_{(0)}]$ , and so on.

The lower convected time derivative is generally denoted by  $[\hat{\sigma}]$  and hence

$$[\hat{\sigma}] = [\bar{\sigma}_{(1)}] \quad (2.55)$$

The material derivative operator  $\frac{D}{Dt}$  is given by

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + (\mathbf{v} \cdot \nabla) = \frac{\partial}{\partial t} + (v_i \frac{\partial}{\partial x_i}) \quad (2.56)$$

We note that the expressions for  $[\bar{\sigma}^{(1)}]$  and  $[\bar{\sigma}_{(1)}]$  contain material derivative plus some more terms, so we can introduce a new notation similar to material derivative and if we drop the over bar on  $[\sigma]$  and super and subscripts [1–9, 13–15], then using (2.41) and (2.50) we can write the following for the contra- and co-variant first convected time derivatives of the corresponding stress tensors.

$$\frac{\nabla}{Dt} [\sigma] = \frac{D}{Dt} [\sigma] - [L][\sigma] - [\sigma][L]^t \quad (2.57)$$

$$\frac{\Delta}{Dt} [\sigma] = \frac{D}{Dt} [\sigma] + [L]^t [\sigma] + [\sigma][L] \quad (2.58)$$

In (2.57) and (2.58) it is understood that  $[\sigma]$  on the right sides of the equations are contra- and co-variant Cauchy stress tensors and the left sides are their first upper convected (contra-variant) and lower convected (co-variant) time derivatives or rates. *Hence forth, we refer to these as upper convected and lower convected stress rates.* Using the new notation in (2.57) and (2.58), we can also define the Jaumann, Truesdell and Green-Naghdi stress rates commonly used in continuum mechanics literature as follows[1–10]

$$\frac{{}^J D[\sigma]}{Dt} = \frac{D}{Dt} [\sigma] - [W][\sigma] + [\sigma][W] \quad (2.59)$$

$$\frac{{}^T D[\sigma]}{Dt} = \frac{D}{Dt} [\sigma] + \text{div}(\mathbf{v})[\sigma] - ([L][\sigma] + [\sigma][L]^t) \quad (2.60)$$

$$\frac{{}^{GN} D[\sigma]}{Dt} = \frac{D}{Dt} [\sigma] - [\Omega][\sigma] + [\sigma][\Omega] \quad (2.61)$$

where  $[\Omega]$  is angular velocity, and  $[W] = \frac{1}{2}([L] - [L]^t)$  is the spin tensor.

#### Remarks:

- (1) Based on the argument presented in the introduction i.e. section 1, it is clear that when the strains are not infinitesimal only contra-variant description is physically justifiable. Thus in case of finite deformation resulting in finite strains, only the upper convected time derivatives (of the contra-variant Cauchy stress tensor) is physical. From (2.57) and (2.58) we clearly note the differences in the convected time derivative expressions in the two cases.

- (2) The derivations of the other stress rates such as Jaumann and Green-Naghdi etc. are possible using (2.57) and (2.58) with modification that are generally justified either based on physical or purely mathematical arguments. Here it suffices to point out that the expression for stress rates in (2.59), (2.61) are not the same as that for upper convected case, hence we expect the deformation behaviors obtained by using these in the constitutive models will undoubtedly deviate from the one resulting by the use of upper convected stress rate.
- (3) It remains to be demonstrated through model problems with theoretical solutions or by performing accurate numerical computations using methods of approximation that: (a) Indeed use of upper convected stress rate in the constitutive models captures the right physics when the deformation is finite. (b) The use of other stress rates in the constitutive models produce spurious behaviors when the strains are no longer infinitesimal. (c) Which rate equations amongst (2.57)- (2.61) remain valid for what magnitude of deformation, is problem dependent. However, from the numerical studies presented in this chapter some inference can be drawn regarding this.
- (4) As pointed out earlier, the lower convected stress rate is a description based on a distorted tetrahedron from that in Figure 5.2 such that the co-variant base vectors are normal to the faces of the new tetrahedron. If we consider upper convected stress rate (2.57) and add  $2[D][\sigma] + 2[\sigma][D]$  to the right side, then if we change the meaning of  $[\sigma]$  to co-variant measure, we can write

$$\frac{\Delta}{Dt}[\sigma] = \frac{D}{Dt}[\sigma] - [L][\sigma] - [\sigma][L]^t + 2[D][\sigma] + 2[\sigma][D] \quad (2.62)$$

$$\text{but } [D] = \frac{1}{2}([L] + [L]^t) \quad (2.63)$$

substituting (2.63) in (2.62)

$$\frac{\Delta}{Dt}[\sigma] = \frac{D}{Dt}[\sigma] + [L]^t[\sigma] + [\sigma][L] \quad (2.64)$$

which is same as (2.58). Thus, the lower convected stress rate requires further deformation or distortion of the deformed tetrahedron shown in Figure 2. We note that the term added to the right side of (2.57) only contains  $[D]$  and not  $[W]$ , hence, the rotation of the actual deformed tetrahedron in Figure 2 is precluded. This deformed configuration of the tetrahedron used in describing the lower convected stress rate is of course non-physical when the deformation is finite.

- (5) It is straight forward to show that Jaumann stress rate is the average of the upper convected (UC) and lower convected (LC) stress rates when the velocity field in UC and LC cases are the same which is only possible if the deformation is not finite. If we define  $[\bar{\sigma}^{(0)}] = [\bar{\sigma}_{(0)}] = [\sigma^J]$ , the Jaumann stress in (2.41) and (2.50) and take their average (i.e. add and divide by two), then we obtain the following

$$\frac{{}^J D[\sigma^J]}{Dt} = \frac{D}{Dt}[\sigma^J] - \frac{1}{2}([L] - [L]^t)[\sigma^J] + [\sigma^J]\frac{1}{2}([L] - [L]^t) \quad (2.65)$$

Substituting for the spin tensor  $[W]$  in terms of velocity gradients and dropping the superscript  $J$  for  $[\sigma^J]$  in (2.65), we obtain

$$\frac{{}^J D[\sigma]}{Dt} = \frac{D}{Dt}[\sigma] - [W][\sigma] + [\sigma][W] \quad (2.66)$$

which is same as the Jaumann stress rate (2.59). It is important to note that  $[\sigma]$  on the right side of (2.66) is neither a contra- nor a co-variant description, it corresponds to an intermediate tetrahedron configuration between those that are used in contra- and co-variant descriptions. We refer to  $[\sigma]$  as Jaumann stress tensor. When the deformation is finite, this description is obviously non-physical.

- (6) Based on the details presented in (4) and (5) and the stress rate expressions for Jaumann and Green-Naghdi rates it is clear that these are neither contra- nor co-variant descriptions. In case of Truesdell rate equation (2.60), we note that it is based on contra-variant basis with the additional term  $div(\mathbf{v})[\sigma]$  that

appears due to consideration of compressibility. If the matter is incompressible and when the velocity field is divergence free, the term  $\text{div}(\mathbf{v})[\sigma]$  is null. For this case, the Truesdell stress rate is same as upper convected. Thus, Truesdell rate is upper convected rate for compressible matter.

### 2.3 Strain measures and convected time derivatives of the strain tensors

In this section we consider strain measures, their material derivatives and the derivations of the convected time derivatives of strain tensors. The contra- and co-variant bases used for defining stress measures and their convected time derivatives naturally suggest the use of same bases in defining strain measures as well as in deriving their convected time derivatives. In continuum mechanics [1–10, 13–15], there are two well accepted and commonly used descriptions of strain measures for finite deformation: the Green strains and the Almansi strains. The Green-strains ( $[\varepsilon]$ ) are co-variant measures while the Almansi strains ( $[\bar{\varepsilon}]$ ) are contra-variant measures. They are defined as [10, 13, 15]

$$[\varepsilon] = \frac{1}{2}([J]^t[J] - [I]) \quad (2.67)$$

$$[\bar{\varepsilon}] = \frac{1}{2}([I] - [\bar{J}][\bar{J}]^t) \quad (2.68)$$

At this point we remark that we have used the definition of  $[\bar{\varepsilon}]$  given by (2.17) as opposed to (2.16) due to the fact that dyads in  $[\bar{\varepsilon}]$  defined by (2.16) are not the right dyads in the  $x$ -frame.  $[\varepsilon]$  and  $[\bar{\varepsilon}]$  in (2.67) and (2.68) have the same dyads that are the correct dyads in the  $x$ -frame.

Consider co-variant description (2.67) and take material derivative of both sides

$$\frac{D}{Dt}[\varepsilon] = \frac{1}{2} \left( \frac{D}{Dt}([J]^t)[J] + [J]^t \frac{D}{Dt}[J] \right) \quad (2.69)$$

Substituting from (2.31)

$$\frac{D}{Dt}[\varepsilon] = \frac{1}{2} ([J]^t[L]^t[J] + [J]^t[L][J]) \quad (2.70)$$

$$\text{or } \frac{D}{Dt}[\varepsilon] = [J]^t \frac{1}{2} ([L]^t + [L])[J] = [J]^t[\gamma_{(0)}][J] \quad (2.71)$$

$$\text{where } [\gamma_{(0)}] = [\gamma_{(1)}] = \frac{1}{2}([L]^t + [L]) \quad (\text{Def.}) \quad (2.72)$$

Let us define

$$[\gamma_{[1]}] = \frac{D}{Dt}[\varepsilon] = [J]^t[\gamma_{(1)}][J] \quad (\text{Def.}) \quad (2.73)$$

$[\gamma_{(0)}]$  is known as the first convected time derivative of the co-variant strain tensor  $[\varepsilon]$ . We can also define higher order convected time derivatives of  $[\varepsilon]$  using a procedure similar to that used earlier in section 2.2 for stresses and using  $[\gamma_{[1]}]$ . For example consider

$$[\gamma_{[2]}] = \frac{D}{Dt}[\gamma_{[1]}] = [J]^t \frac{D}{Dt}([\gamma_{(1)}])[J] + \frac{D}{Dt}([J]^t)[\gamma_{(1)}][J] + [J]^t[\gamma_{(1)}] \frac{D}{Dt}[J] \quad (2.74)$$

Substituting from (2.31) into (2.74), rearranging and grouping terms

$$[\gamma_{[2]}] = \frac{D}{Dt}[\gamma_{[1]}] = [J]^t \left( \frac{D}{Dt}[\gamma_{(1)}] + [L]^t[\gamma_{(1)}] + [\gamma_{(1)}][L] \right) [J] \quad (2.75)$$

Let

$$[\gamma_{(2)}] = \frac{D}{Dt}[\gamma_{(1)}] + [L]^t[\gamma_{(1)}] + [\gamma_{(1)}][L] \quad (\text{Def.}) \quad (2.76)$$

Hence

$$[\gamma_{[2]}] = [J]^t[\gamma_{(2)}][J] \quad (\text{Def.}) \quad (2.77)$$

$[\gamma_{(2)}]$  is the second convected time derivatives of the co-variant strain tensor  $[\varepsilon]$ . This procedure can be used to obtain convected time derivatives of co-variant strain tensor  $[\varepsilon]$  of any desired order.

Next, we consider contra-variant strain description (2.68) and take its material derivative

$$\frac{D}{Dt}[\bar{\varepsilon}] = -\frac{1}{2} \left( \frac{D}{Dt}([\bar{J}])[\bar{J}]^t + [\bar{J}] \frac{D}{Dt}[\bar{J}]^t \right) \quad (2.78)$$

Substituting from (2.37) in (2.78) and defining  $[\gamma^{[1]}]$

$$[\gamma^{[1]}] = \frac{D}{Dt}[\bar{\varepsilon}] = \frac{1}{2} ([\bar{J}][L][\bar{J}]^t + [\bar{J}][L]^t[\bar{J}])$$

or

$$[\gamma^{[1]}] = \frac{D}{Dt}[\bar{\varepsilon}] = [\bar{J}] \frac{1}{2} ([L] + [L]^t) [\bar{J}]^t = [\bar{J}] [\gamma^{(0)}] [\bar{J}]^t \quad (2.79)$$

$$\text{where } [\gamma^{(0)}] = [\gamma^{(1)}] = \frac{1}{2} ([L] + [L]^t) \quad (\text{Def.}) \quad (2.80)$$

$[\gamma^{(0)}]$  is known as the first convected time derivative of the contra-variant strain tensor  $[\bar{\varepsilon}]$ . We note that  $[\gamma^{(1)}] = [\gamma^{(1)}]$ . We can also define higher order convected time derivatives of  $[\bar{\varepsilon}]$  using a procedure similar to that used for co-variant case. For example consider

$$[\gamma^{[2]}] = \frac{D}{Dt}[\gamma^{[1]}] = \frac{D}{Dt}([\bar{J}][\gamma^{(1)}][\bar{J}]^t) \quad (2.81)$$

$$[\gamma^{[2]}] = [\bar{J}] \frac{D}{Dt}([\gamma^{(1)}])[\bar{J}]^t + \frac{D}{Dt}([\bar{J}])[\gamma^{(1)}][\bar{J}]^t + [\bar{J}][\gamma^{(1)}] \frac{D}{Dt}[\bar{J}]^t \quad (2.82)$$

Substituting from (2.37) in (2.82), rearranging and regrouping terms

$$[\gamma^{[2]}] = [\bar{J}] \left( \frac{D}{Dt}[\gamma^{(1)}] - [L][\gamma^{(1)}] - [\gamma^{(1)}][L]^t \right) [\bar{J}]^t \quad (2.83)$$

Let

$$[\gamma^{(2)}] = \frac{D}{Dt}[\gamma^{(1)}] - [L][\gamma^{(1)}] - [\gamma^{(1)}][L]^t \quad (\text{Def.}) \quad (2.84)$$

Hence

$$[\gamma^{[2]}] = [\bar{J}][\gamma^{(2)}][\bar{J}]^t \quad (\text{Def.}) \quad (2.85)$$

$[\gamma^{(2)}]$  is the second convected time derivatives of the contra-variant strain tensor  $[\bar{\varepsilon}]$ . This procedure can be used to obtain contra-variant convected time derivatives of tensor  $[\bar{\varepsilon}]$  of any desired order.

## 2.4 Constitutive equations

### General and theoretical considerations

In the development of the mathematical models for deforming matter based on conservation laws, the constitutive equations describing the constitution of the matter are essential to provide closure to the mathematical models and to incorporate material specific physics in the mathematical models derived using conservation laws. The constitutive equations must satisfy certain physical and mathematical requirements. Based on [1, 2, 7, 8], the principles of casualty, determinism, equipresence, objectivity, material invariance, neighborhood, memory and admissibility are fundamental in the development of the constitutive relations for the matter. In general, for a thermo-mechanical process the constitutive equation: (1) must describe how heat flux is related to temperature gradients and conductivity. This is adequately described by Fourier heat conduction law. (2) must describe a relationship between stresses and deformation. This aspect is considered in this chapter. A detailed discussion of all of the principles is beyond the scope of this chapter. Instead we only elaborate on two principles that are most relevant in view of the work considered in this chapter: (1) The principle of material objectivity or frame invariance. The constitutive equation must be form-invariant with respect to rigid motions of the spatial frame of reference i.e. the form of the constitutive equations should not change due to rigid translation and rotation of the spatial frame of reference. (2) The principle of admissibility. According to the principle of admissibility all constitutive equations must be consistent with the basic principles of continuum mechanics, that is, they are subjected to the principles of conservation of mass, balance of momenta,

conservation of energy (first law of thermodynamics), and the Clausius-Duhem inequality (second law of thermodynamics). The first three conservation laws yield well known continuity, momentum and energy equations. The second law of thermodynamics yields a set of conditions that must be satisfied to ensure thermodynamics equilibrium of deforming matter. These conditions establish dependence of Helmholtz free energy on scalars, vectors and tensors describing the deformation and provide information regarding heat flux and temperature gradient among others. The specific form of these conditions vary depending upon the assumed physics of the deforming matter.

Since in this chapter we only consider Eulerian descriptions of the deforming matter, the dependent variables of choice are velocities (among others) instead of displacements. The material particle displacements in such description are not known. Thus, instead of displacement gradients, we have velocity gradients. Hence, the development of the constitutive equations can not utilize strain measures (as they require displacement gradients) but instead must consider the use of velocity gradients or strain rates. Thus, all constitutive equations in Eulerian descriptions are rate constitutive equations in which convected time derivatives of order zero or one of the chosen stress tensor are expressed in terms of the convected time derivatives of order zero or higher of the chosen strain tensor and other arguments and the properties of the deforming matter. In the development of the constitutive equations in Eulerian description for solids as well as fluids it is fundamental to decompose the total stress tensor  $[\bar{\sigma}]$  (can be in contra- or co-variant basis) into equilibrium stress  $[{}_e\bar{\sigma}]$  and deviatoric stress  $[{}_d\bar{\sigma}]$ .

$$[\bar{\sigma}] = [{}_e\bar{\sigma}] + [{}_d\bar{\sigma}] \quad (2.86)$$

In case of compressible matter  $[{}_e\bar{\sigma}]$  can be derived directly using Clausius-Duhem inequality and Helmholtz free energy [7, 8].

$$[{}_e\bar{\sigma}] = -p(\bar{\rho}, \theta)[I] \quad (2.87)$$

where  $p(\bar{\rho}, \theta)$  is thermodynamic pressure and is defined by equation of state and is assumed positive when compressive.  $\bar{\rho}$  and  $\theta$  are density and temperature in the current configuration. Thus in this case the thermodynamic pressure is deterministic from the deformation field of the matter. If the matter is incompressible then  $|J| = 1$  condition must be satisfied. This condition in conjunction with Clausius-Duhem inequality yields

$$[{}_e\bar{\sigma}] = -p[I] \quad (2.88)$$

in which  $p$  is mechanical pressure and is also assumed positive when compressive. Mechanical pressure  $p$  can not be determined by the deformation field. we remark that (2.86)- (2.88) hold regardless of whether the deforming matter is a solid or a fluid. Thus, to define  $[\bar{\sigma}]$  in (2.86), we must describe how  $[{}_d\bar{\sigma}]$  is related to the various measures describing the deformation of the matter. These indeed are rate constitutive equations regardless of whether the matter is a solid or a fluid. We remark that the condition resulting from the Clausius-Duhem inequality for establishing constitutive equations for  $[{}_d\bar{\sigma}]$  only requires that conversion of mechanical energy (viscous dissipation) due to  $[{}_d\bar{\sigma}]$  be positive but provides no other means to establish the explicit forms of the constitutive equations for  $[{}_d\bar{\sigma}]$ . This leaves the approach of developing rate constitutive equations wide open to entertain many possible alternatives. Thus the rate constitutive equation in general have no thermodynamic foundation (also see [7, 8, 10]). However, some continuum mechanics principles, if utilized systematically may provide a more rational basis for the development of the rate constitutive equations. We consider some important aspect that are crucial in the development of the rate constitutive equations and are pertinent in establishing their ability to describe the physics of the deforming matter (even though there is lack of thermodynamic basis) for progressively increasing deformation.

- (a) The most convenient way to derive the rate constitutive equations is to consider convected coordinate system defining the deformed material lines in the current configuration (see section 1).
- (b) In the convected coordinate system, there are two obvious ways to define measures of stresses, strains and their convected time derivatives (derived in section 2.2 and 2.3): contra-variant basis or co-variant basis. The development of the constitutive relations requires development of relationships between the convected time derivatives of the chosen measures of stresses and strains and the properties of the matter as well as other tensors and vectors influencing the stress field. For this purpose:
  - (i) The first important consideration is to choose compatible conjugate pairs of convected time derivatives of the stress and strain tensors. The choices based on the contra- and co-variant measures are

rather obvious. The convected time derivatives of both stress and strain tensors must have the same basis i.e. either contra- or co-variant. Thus  $[_d\bar{\sigma}^{(i)}], [\gamma^{(i)}]; i = 0, 1, \dots$  are compatible and likewise so are  $[_d\bar{\sigma}_{(i)}], [\gamma_{(i)}]; i = 0, 1, \dots$

- (ii) The second important consideration is to ensure that the convected time derivatives of the compatible pairs of stress and strain tensors are objective or frame invariant. It is rather straight forward to show that convected time derivatives of all orders of the stress and the strain tensors derived and/or presented in section 2.2 and 2.3 are indeed objective or frame invariant (proofs omitted for the sake of brevity).
  - (iii) A principle is needed that will allow us to relate the convected time derivatives of the chosen stress tensor to the convected time derivatives of the chosen strain tensor and other measures influencing stress and the properties of the matter. We remark that Clausius-Duhem inequality in this case only requires that viscous dissipation be positive but provides no other means that can be used to established the explicit forms of the constitutive equations.
- (c) Since the Clausius-Duhem inequality does not provide a mechanism for establishing rate constitutive equation for defining stress field  $[_d\bar{\sigma}]$  (contra- or co-variant bases), we need to consider another alternative. If we examine the development of constitutive equation for solid elastic matter in Lagrangian description, then we find that in this case the constitutive equations are strictly deterministic from the Clausius-Duhem inequality and Helmholtz free energy. We find that the constitutive equations for the stress tensor are in fact a linear combination of the generators of the conjugate strain tensor. This observation suggest that if we can determine the dependence of the first convected derivative of  $[_d\bar{\sigma}]$  on tensors and vectors defining the physics of deforming matter then we can express the first convected derivative of the  $[_d\bar{\sigma}]$  in terms of a linear combination of the combined generators (of the same rank as  $[_d\bar{\sigma}]$ ) of the tensors and vectors in its argument [7, 8, 10, 16–26]. The coefficients involved in the linear combination are functions of the combined invariants of the tensors and vectors in its argument as well as temperature. The final coefficients in the constitutive equations are established by using Taylor series expansion of the coefficients in the linear combination about the reference configuration [10, 27–29]. We consider various rate constitutive equations in the following.

### Various rate constitutive equations

#### (a) *Compressible viscous Newtonian fluids (homogeneous, isotropic)*[10, 27]

We consider these to be thermoviscous fluids.

*Contra-variant basis:* Consider  $[_d\bar{\sigma}^{(0)}]$ , convected time derivative of order zero of the contra-variant deviatoric stress. If we assume that

$$[_d\bar{\sigma}^{(0)}] = [_d\bar{\sigma}^{(0)}]([D], \theta) = [_d\bar{\sigma}^{(0)}](\gamma^{(0)}, \theta) = [_d\bar{\sigma}^{(0)}](\gamma^{(1)}, \theta) \quad (2.89)$$

then in this case the generators are  $[I], [\gamma^{(0)}], [\gamma^{(0)}]^2$  and the principal invariants are  $i_{\gamma^{(0)}} = \text{tr}[\gamma^{(0)}]$ ,  $ii_{\gamma^{(0)}} = \text{tr}([\gamma^{(0)}]^2)$  and  $iii_{\gamma^{(0)}} = \text{tr}([\gamma^{(0)}]^3)$ .

$$\therefore [_d\bar{\sigma}^{(0)}] = C_0[I] + C_1[\gamma^{(0)}] + C_2[\gamma^{(0)}]^2 \quad (2.90)$$

$$C_i = C_i(i_{\gamma^{(0)}}, ii_{\gamma^{(0)}}, iii_{\gamma^{(0)}}, \theta) \quad ; \quad i = 0, 1, 2 \quad (2.91)$$

Expanding  $C_i$  in Taylor series about the reference configuration and considering only first order theory (i.e. squares, products and higher order terms in  $[\gamma^{(0)}]$  are neglected) and then substituting them in (2.90) yields (if thermal expansion is neglected and the reference configuration is assumed stress free)

$$[_d\bar{\sigma}^{(0)}] = 2\eta[\gamma^{(0)}] + \kappa\text{tr}[\gamma^{(0)}][I] = 2\eta[\gamma^{(1)}] + \kappa\text{tr}[\gamma^{(1)}][I] \quad (2.92)$$

If we redefine  $[_d\bar{\sigma}^{(0)}] = [\bar{\tau}^{(0)}]$ , viscous stress in contra-variant basis, then

$$[\bar{\tau}^{(0)}] = 2\eta[\gamma^{(0)}] + \kappa\text{tr}[\gamma^{(0)}][I] \quad (2.93)$$

This is Newton's law of viscosity for a compressible fluid in which  $\eta$  is viscosity and  $\kappa$  is second viscosity and the viscous stress is contra-variant measure.

*Co-variant basis:* Consider  $[_d\bar{\sigma}_{(0)}]$ , convected time derivative of order zero of the co-variant deviatoric stress. If we assume that

$$[_d\bar{\sigma}_{(0)}] = [_d\bar{\sigma}_{(0)}]([D], \theta) = [_d\bar{\sigma}_{(0)}]([\gamma_{(0)}], \theta) = [_d\bar{\sigma}_{(0)}]([\gamma_{(1)}], \theta) \quad (2.94)$$

then following the contra-variant case, we can write

$$[_d\bar{\sigma}_{(0)}] = \hat{C}_0[I] + \hat{C}_1[\gamma_{(0)}] + \hat{C}_2[\gamma_{(0)}]^2 \quad (2.95)$$

Following the procedure similar to contra-variant basis, we obtain the following (assuming that thermal expansion is neglected and the reference configuration is stress free)

$$[_d\bar{\sigma}_{(0)}] = 2\eta[\gamma_{(0)}] + \kappa \text{tr}[\gamma_{(0)}][I] = 2\eta[\gamma_{(1)}] + \kappa \text{tr}[\gamma_{(1)}][I] \quad (2.96)$$

or

$$[\bar{\tau}_{(0)}] = 2\eta[\gamma_{(0)}] + \kappa \text{tr}[\gamma_{(0)}][I] \quad (2.97)$$

$[\bar{\tau}_{(0)}]$  is viscous stress in co-variant basis.

Since  $[\gamma_{(0)}] = [\gamma^{(0)}] = [D]$ , right sides of (2.93) and (2.97) are identical, thus  $[\bar{\tau}_{(0)}] = [\bar{\tau}^{(0)}] = [\bar{\tau}]$ , hence for viscous Newtonian compressible fluids the contra-and co-variant descriptions are same and we can write

$$[\bar{\tau}] = 2\eta[D] + \kappa \text{tr}[D][I] \quad (2.98)$$

(2.98) is well known expression for viscous stress tensor for compressible viscous Newtonian fluids. We remark that these are rate constitutive equations employing convected time derivatives of order zero of stress and strain measures (The strain measure being Almansi strain or Green's strain).

#### **(b) Incompressible viscous Newtonian fluids**

In this case  $\text{tr}[\gamma^{(0)}] = \text{tr}[\gamma_{(0)}] = \text{tr}[D] = 0$ , hence (2.98) reduces to

$$[\bar{\tau}] = 2\eta[D] \quad (2.99)$$

#### **Remarks:**

- (1) Derivations in (a) and (b) employ theory of generators and invariants and do not use Clausius-Duhem inequality as it provides no mechanism for deriving these.
- (2) For (2.98) and (2.99) to be thermodynamically admissible, the Clausius-Duhem inequality requires that viscous dissipation due to  $[\bar{\tau}]$  must be positive. However, the Clausius-Duhem inequality i.e. second law of thermodynamic provides no mechanism for their derivation.
- (3) The derivation employs theory of generators and invariants and hence has a foundation from the point of view of continuum mechanics principles.
- (4) We observe that in this case contra- and co-variant descriptions are same, hence the rate constitutive equations are unique and same regardless of the choice of convected coordinate system.

#### **(c) Incompressible elastic matter:**

Details of the derivations of these rate constitutive equations based on the theory of generators and invariants and discussion of their thermodynamics admissibility for solid matter were presented in chapter 3 and can also be found in [10]. Here we simply summarize the results based on first order theory i.e. assuming that stress rates are a linear function of the generators of the argument tensors. We also neglect thermal effects. To simplify the notations, we use  $[_d\bar{\sigma}^{(1)}] = [\bar{\tau}^{(1)}]$  and  $[_d\bar{\sigma}_{(1)}] = [\bar{\tau}_{(1)}]$  etc.. Further more, since the upper convected, lower convected, Jaumann etc. stress rates are indicated by the objective derivative symbols and Eulerian description

is understood, we can drop over bar on  $[\tau]$  as well as super and subscript  $'(1)'$ . Thus, in the following we use  $[\tau]$  for stress which in fact is the deviatoric component. Using the definitions of convected derivatives of stress tensor  $[\sigma]$  defined in section 2.2 and replacing  $[\sigma]$  by  $[\tau]$  and keeping in mind that  $[\tau]$  is the deviatoric part of the stress tensor, we have the following rate constitutive equations for solid elastic matter defining rates of  $[\tau]$ . Details of the derivations are presented in reference [10, 28].

*Contra-variant basis : Upper convected rate constitutive equations*

$$[\tau^{(1)}] = \frac{\nabla}{Dt}[\tau] = 2\mu\gamma^{(1)} \quad (2.100)$$

where  $\mu$  is the shear modulus. In this case the  $[\tau^{(1)}]$ ,  $[\gamma^{(1)}]$  are compatible first convected time derivative in contra-variant basis. (2.100) utilizes contra-variant basis corresponding to the true deformed current configuration (tetrahedron in Figure 5.2). The contra-variant base vectors normal to the tetrahedron faces in the current configuration is the most natural and physical for the stress and strain descriptions and their convected time derivatives. Both  $[\tau^{(1)}]$  and  $[\gamma^{(1)}]$  are objective or frame invariant i.e. the form of (2.100) does not change upon rigid rotation of the spatial frame of reference. There are no undue or anomalous assumptions or approximations in the derivation other than the assumption of the first order theory.

*Co-variant basis : Lower convected rate constitutive equations*

The rate constitutive equation in this case utilize compatible pairs  $[\tau_{(1)}]$  and  $[\gamma_{(1)}]$  and we can write

$$[\tau_{(1)}] = \frac{\Delta}{Dt}[\tau] = 2\mu\gamma_{(1)} \quad (2.101)$$

since  $[\gamma_{(1)}] = [\gamma^{(1)}]$ , the right hand side of (2.100) and (2.101) are identical. As mentioned and shown earlier, we again remark that co-variant basis utilizes a non-physical deformed configuration i.e. a tetrahedron obtained by further deformation of the actual deformed tetrahedron shown in Figure 5.2. This is obviously non-physical. As the magnitudes of the deformation increases, the contra- and co-variant base vectors directions no longer remain parallel. Thus, with progressively increasing deformation (2.101) can be expected to produce progressively non-physical behavior.

*Jaumann rate constitutive equations*

As shown in section 2.2, the first convected time derivative of the Jaumann stress tensor is in fact average of  $[\tau^{(1)}]$  and  $[\tau_{(1)}]$  when the velocity field is same in both UC and LC cases. Thus, it utilizes a deformed configuration in between the contra- and the co-variant configurations. Therefore, the choice of a compatible (or conjugate) first convected time derivative of the strain tensor is not straight forward. But, if we assume that  $[\gamma^{(1)}] = [\gamma_{(1)}]$  holds for all intermediate configurations of the tetrahedron between contra- and co-variant cases, then, we can write

$$\frac{^J D[\tau]}{Dt} = 2\mu\gamma^{(1)} = 2\mu\gamma_{(1)} \quad (2.102)$$

The fact that  $[\gamma_{(1)}] = [\gamma^{(1)}]$  is assumed to hold for all configurations between contra- and co-variant configurations, right side of (2.102) is obviously same as those of (2.100) and (2.101). Since the rate equations in co-variant basis are non-physical, so are (2.102) when the deformation is finite for which case the strain deviates from the infinitesimal assumption.

*Truesdell rate constitutive equations*

The Truesdell rate constitutive equations are upper convected rate constitutive equations for compressible matter [10], hence we can write the following:

$$\frac{^T D[\tau]}{Dt} = 2\mu\gamma^{(1)} \quad (2.103)$$

If the velocity field in the deforming matter is divergence free then  $\text{div}(\mathbf{v})[\tau]$  term is null and hence in this case (2.103) is identical to upper convected rate constitutive equations (2.100) for incompressible matter.

**Remarks:**

- (1) Many of the remarks presented in section 2.2 regarding convected time derivatives of the stress tensor remain valid for the rate constitutive equations primarily because the convected time derivatives defined in section 2.2 have been used in constructing the rate constitutive equations.
- (2) The upper convected rate constitutive equations are based on actual deformed tetrahedron for the definitions of stress and strain tensors and their convected time derivatives. The contra-variant basis is physical and leads to mathematically rigorous derivation.
- (3) All other rate constitutive equations (except Truesdell) utilize deformed tetrahedron configurations to define stress and strain tensors and their convected time derivatives, which are non-physical when infinitesimal strain assumption is violated and hence are expected to become increasingly spurious with progressively increasing deformation and strains. The severity of the anomalous behaviors may be model problem (i.e. physics) dependent.
- (4) A fundamental aspect of the different rate constitutive equations is that they utilize different definitions of the stress tensor and its first convected time derivative.

**Rate constitutive equations for viscoelastic polymeric liquids**

In this section we consider rate constitutive equations for incompressible viscoelastic polymeric liquids. These liquids have viscosity as well as elasticity. We consider constitutive models for dilute polymeric liquids such as Maxwell model, Oldroyd-B model as well as those for polymer melts such as Giesekus model. These constitutive models utilize stress measure, its first convected time derivative and convected time derivatives of strain measure in an appropriately chosen basis and the constitution of the matter i.e. properties of the polymeric liquid. Since the main thrust of this work is the investigation of the behaviors of various rate constitutive equations in the mathematical models, we simply present commonly used rate constitutive equations for polymeric liquids without detailed derivations. First, we decompose the total stress tensor  $[\sigma]$  into pressure  $p$  (assumed positive when compressive) and a stress tensor  $[\tau]$  due to viscosity and elasticity of the polymer.

$$\sigma_{ij} = -p\delta_{ij} + \tau_{ij} \quad (2.104)$$

furthermore, we assume that

$$[\tau] = [\tau^p] + [\tau^s] \quad (2.105)$$

and

$$[\tau^p] = [\tau^{pv}] + [\tau^e] \quad (2.106)$$

in which  $s, p, pv$  and  $e$  stand for solvent, polymer, polymer viscous and elastic. Also we note that

$$[\tau^s] = 2\eta_s[D] = 2\eta_s[\gamma^{(1)}] = 2\eta_s[\gamma_{(1)}] \quad (2.107)$$

$$[\tau^{pv}] = 2\eta_p[D] = 2\eta_p[\gamma^{(1)}] = 2\eta_p[\gamma_{(1)}] \quad (2.108)$$

$\eta_s$  and  $\eta_p$  are solvent and polymer viscosities.

The rate constitutive equations for dilute polymeric liquids such as Maxwell and Oldroyd-B constitutive equations are presented using  $[\tau]$  whereas Giesekus constitutive model for polymer melts is presented using  $[\tau^p]$  (see reference [14]). These are all Eulerian descriptions. Overbar (-) on all quantities has been omitted for simplicity of notations. In the following we assume isothermal case.

**Dilute viscoelastic polymeric liquids**

The Maxwell model and the Oldroyd-B model are commonly used rate constitutive models for dilute polymeric liquids.

*Maxwell rate constitutive equations:*

Using contra-variant, co-variant, Jaumann and Truesdell stress measures and their first convected time derivative we can write the following for the upper convected, lower convected, Jaumann and Truesdell rate constitutive equations for the Maxwell model for dilute polymeric liquids (derivations are presented in reference [29]).

$$\boldsymbol{\tau}^{(0)} + \lambda_1 \boldsymbol{\tau}^{(1)} = 2\eta_0 \boldsymbol{\gamma}^{(1)} \quad (2.109)$$

$$\boldsymbol{\tau}_{(0)} + \lambda_1 \boldsymbol{\tau}_{(1)} = 2\eta_0 \boldsymbol{\gamma}_{(1)} \quad (2.110)$$

$$\boldsymbol{\tau} + \lambda_1 \frac{^J D \boldsymbol{\tau}}{Dt} = 2\eta_0 \boldsymbol{\gamma}^{(1)} \quad (2.111)$$

$$\boldsymbol{\tau} + \lambda_1 \frac{^T D \boldsymbol{\tau}}{Dt} = 2\eta_0 \boldsymbol{\gamma}^{(1)} \quad (2.112)$$

In (2.111) and (2.112),  $\boldsymbol{\tau}$  is obviously Jaumann and Truesdell stress tensor. These constitutive equations are referred to as linear visco-elastic model.  $\eta_0$  is zero shear rate viscosity and  $\lambda_1$  is relaxation time.

*Oldroyd-B rate constitutive equations:*

Oldroyd-B rate constitutive equations describe quasilinear differential constitutive model for dilute polymeric liquids. Parallel to Maxwell model, here we have (See reference [29] for derivation)

$$\boldsymbol{\tau}^{(0)} + \lambda_1 \boldsymbol{\tau}^{(1)} = 2\eta_0 (\boldsymbol{\gamma}^{(1)} + \lambda_2 \boldsymbol{\gamma}^{(2)}) \quad (2.113)$$

$$\boldsymbol{\tau}_{(0)} + \lambda_1 \boldsymbol{\tau}_{(1)} = 2\eta_0 (\boldsymbol{\gamma}_{(1)} + \lambda_2 \boldsymbol{\gamma}_{(2)}) \quad (2.114)$$

$$\boldsymbol{\tau} + \lambda_1 \frac{^J D \boldsymbol{\tau}}{Dt} = 2\eta_0 [\boldsymbol{\gamma}^{(1)} + \frac{\lambda_2}{2} (\boldsymbol{\gamma}^{(2)} + \boldsymbol{\gamma}_{(2)})] \quad (2.115)$$

$$\boldsymbol{\tau} + \lambda_1 \frac{^T D \boldsymbol{\tau}}{Dt} = 2\eta_0 (\boldsymbol{\gamma}^{(1)} + \lambda_2 \boldsymbol{\gamma}^{(2)}) \quad (2.116)$$

(2.113) - (2.116) are upper convected, lower convected, Jaumann and Truesdell rate constitutive equations based on Oldroyd-B model for dilute polymeric liquids.  $\lambda_2$  is retardation time.

#### **Polymer melts: Giesekus constitutive model**

This model is primarily used for dense polymers or polymer melts in which the viscoelastic polymeric liquid behavior is elastically dominated. The Giesekus constitutive model using various measures of the stress and their convected time derivatives can be defined as (See reference [29] for derivation),

$$(\boldsymbol{\tau}^p)^{(0)} + \lambda_1 \boldsymbol{\tau}^{p(1)} + \alpha \frac{\lambda_1}{\eta_p} (\boldsymbol{\tau}^p)^{(0)} (\boldsymbol{\tau}^p)^{(0)} = 2\eta_p \boldsymbol{\gamma}^{(1)} \quad (2.117)$$

$$(\boldsymbol{\tau}^p)_{(0)} + \lambda_1 \boldsymbol{\tau}^p_{(1)} + \alpha \frac{\lambda_1}{\eta_p} (\boldsymbol{\tau}^p)_{(0)} (\boldsymbol{\tau}^p)_{(0)} = 2\eta_p \boldsymbol{\gamma}_{(1)} \quad (2.118)$$

$$(\boldsymbol{\tau}^p) + \lambda_1 \frac{^J D \boldsymbol{\tau}^p}{Dt} + \alpha \frac{\lambda_1}{\eta_p} (\boldsymbol{\tau}^p) (\boldsymbol{\tau}^p) = 2\eta_p \boldsymbol{\gamma}_{(1)} \quad (2.119)$$

$$(\boldsymbol{\tau}^p) + \lambda_1 \frac{^T D \boldsymbol{\tau}^p}{Dt} + \alpha \frac{\lambda_1}{\eta_p} (\boldsymbol{\tau}^p) (\boldsymbol{\tau}^p) = 2\eta_p \boldsymbol{\gamma}^{(1)} \quad (2.120)$$

(2.117) - (2.120) are upper convected, lower convected, Jaumann and Truesdell rate constitutive equations based on Giesekus model.  $\alpha$  is called mobility factor and  $\eta_p$  is polymer viscosity.

#### **Remarks:**

- (1) In this section we have presented commonly used rate constitutive equation for polymeric liquids (dense as well dilute) without their derivations.

- (2) Literature review on the development of these rate equations and reference [14] suggest various approaches for their derivations and justifications for their validity from engineering point of view.
- (3) Our view is that the published work on the derivations of the rate constitutive equation for polymeric liquids lacks continuum mechanics foundation and a general framework.
- (4) In chapter 4 we present a general framework for deriving rate constitutive equation for thermoviscoelastic polymeric liquids based on theory of generators and invariants as well discuss their admissibility within the thermodynamic framework of continuum mechanics.
- (5) Since our thrust in this chapter is to demonstrate the basis (contra-, co-variant or other) behind the rate constitutive equations and their validity for finite deformation, we have simply presented the final forms of the rate constitutive equations that are commonly used and have given some discussion of their validity based on physics of the deforming matter. Numerical studies substantiate these points quite well.

### 3 General considerations for numerical studies

In reference [12] numerical studies were presented for wave propagation in solid linear elastic material for progressively increasing strains to demonstrate that only upper convected rate constitutive equations produce physically meaningful results when the strains begin to deviate from infinitesimal assumption. In these studies, use of linear elastic material behavior assumption (with modulus of elasticity  $E$  and Poisson's ratio  $\nu$ ) perhaps raises the issue of their validity in terms of incorporating the correct physics for finite strains. These studies were duplicated and are confirmed to be in agreement with those presented in reference [12] but are not presented in this report.

As shown in the theoretical development, the major issue in this work is to demonstrate the validity or lack validity of the various convected time derivatives of the stress measure in the rate constitutive equations, hence any rate constitutive model that utilize these would suffice. We choose Giesekus constitutive model to conduct studies for progressively increasing strain and strain rates to illustrate the behaviors of various rate constitutive equations.

### 4 Obtaining solutions of model problem(s)

Even for simplest possible flow such as fully developed flow between parallel plates, the BVP or the IVP described by the mathematical model resulting from the conservation laws and the Giesekus constitutive model does not permit theoretical solution. These are a system of non-linear PDEs in the dependent variables, spatial coordinates and time. Their solutions must be obtained numerically using methods of approximation. Based on reference [30, 31], the space-time coupled least square finite element process using space-time strip or slab with time marching in *hpk*-mathematical and computational framework [32–34] is an ideal method of approximation for obtaining the numerical solution of the IVPs associated with the mathematical model. In case of BVPs, the least square finite element method in *hpk* framework [32–34] is the best choice.

We consider fully developed flow of a Giesekus fluid between parallel plates. The mathematical model describing the physics of the flow is a system of non-linear PDEs in the dependent variables, a BVP. For such BVPs, the least square finite element processes yield variationally consistent integral forms [32–34] that ensure symmetric and positive definite coefficient matrices unconditionally. *hpk* mathematical and computational framework permits higher order global differentiability in the entire computational process and all integrals can be maintained in the Riemann sense. This permits accurate computations of the desired  $L_2$ -norms,  $\sqrt{I} = \sqrt{\sum_i (E_i, E_i)}$  of the residuals, and  $E_i$ , the residuals resulting from the non-discretized governing differential equations. When  $I \rightarrow 0$ , we are assured that  $E_i \rightarrow 0$  i.e. GDEs are satisfied accurately over the entire domain of definition of the BVP in the pointwise sense. In all numerical studies, low value of  $I$  ( $O(10^{-8})$  or lower) is sought to ensure that GDEs are satisfied accurately. Details of the least square finite element method for BVPs in *hpk* framework can be found in reference [32–34].

## 5 Model problem: fully developed flow of a Giesekus fluid between parallel plates

For this model problem, the mathematical model results in a BVP. Assuming the polymeric liquid to be incompressible and the flow to be isothermal, the continuity equation is satisfied identically and the energy equation is not needed. Thus, the mathematical model consists of the momentum equations and the appropriately chosen constitutive equations.

### 5.1 Mathematical model

Since the Giesekus constitutive model is derived using polymer stresses ( $\tau^p$ ), the most suitable choice of dependent variables is velocities, polymer stresses and pressure ( $p$ ). We use hat ( $\hat{\cdot}$ ) on all quantities to emphasize that all quantities have their appropriate dimensions in terms of force, length and time. Consider the schematic shown in Figure 4, where  $H$  is half of the distance between the parallel plates.

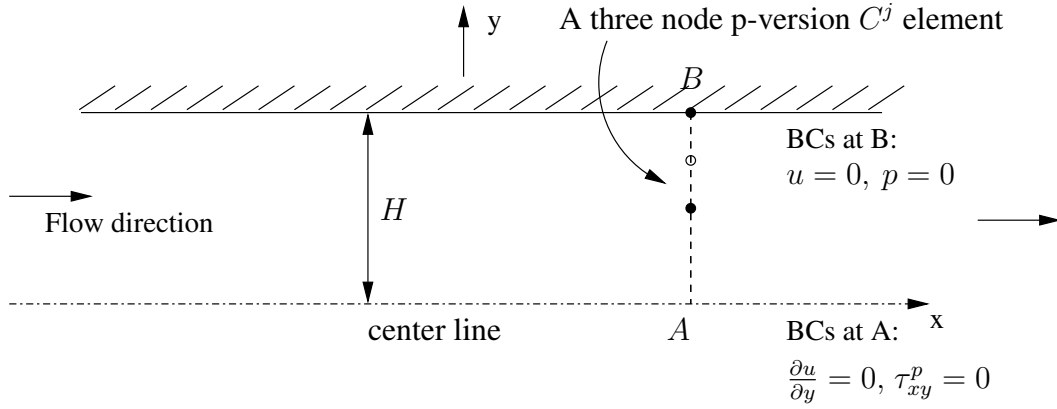


Figure 5.4: Schematic of 1-D fully developed flow between parallel plates (half domain)

*Momentum equations:*

In the absence of body forces, the momentum equations are given by (remain the same regardless of the choice of rate constitutive equations).

$$\frac{\partial \hat{p}}{\partial \hat{x}} - \left( \frac{\partial \hat{\tau}_{xy}^p}{\partial \hat{y}} + \hat{\eta}_s \frac{\partial^2 \hat{u}}{\partial \hat{y}^2} \right) = 0 \quad (5.1)$$

$$\frac{\partial \hat{p}}{\partial \hat{y}} - \frac{\partial \hat{\tau}_{yy}^p}{\partial \hat{y}} = 0 \quad (5.2)$$

We note that the stresses  $\hat{\tau}^p$  are upper convected or lower convected or Jaumann or Truesdell depending upon the choice of the rate constitutive equations.

*Rate constitutive equations:*

Explicit forms of the rate constitutive equations for upper convected, lower convected, Jaumann and Truesdell stress rates are given in the following.

*Upper convected:*

If  $\hat{\tau}^p$  is the contra-variant Cauchy stress tensor then, we have

$$\hat{\tau}_{xx}^p - 2\lambda_1 \hat{\tau}_{xy}^p \frac{\partial \hat{u}}{\partial \hat{y}} + \alpha \frac{\lambda_1}{\hat{\eta}_p} ((\hat{\tau}_{xx}^p)^2 + (\hat{\tau}_{xy}^p)^2) = 0 \quad (5.3)$$

$$\hat{\tau}_{yy}^p + \alpha \frac{\lambda_1}{\hat{\eta}_p} ((\hat{\tau}_{xy}^p)^2 + (\hat{\tau}_{yy}^p)^2) = 0 \quad (5.4)$$

$$\hat{\tau}_{xy}^p - \lambda_1 \hat{\tau}_{yy}^p \frac{\partial \hat{u}}{\partial \hat{y}} + \alpha \frac{\lambda_1}{\hat{\eta}_p} \hat{\tau}_{xy}^p (\hat{\tau}_{xx}^p + \hat{\tau}_{yy}^p) - \hat{\eta}_p \frac{\partial \hat{u}}{\partial \hat{y}} = 0 \quad (5.5)$$

*Lower convected:*

If  $\hat{\tau}^p$  is the co-variant Cauchy stress tensor then, we have

$$\hat{\tau}_{xx}^p + \alpha \frac{\lambda_1}{\hat{\eta}_p} ((\hat{\tau}_{xx}^p)^2 + (\hat{\tau}_{xy}^p)^2) = 0 \quad (5.6)$$

$$\hat{\tau}_{yy}^p + 2\lambda_1 \hat{\tau}_{xy}^p \frac{\partial \hat{u}}{\partial \hat{y}} + \alpha \frac{\lambda_1}{\hat{\eta}_p} ((\hat{\tau}_{xy}^p)^2 + (\hat{\tau}_{yy}^p)^2) = 0 \quad (5.7)$$

$$\hat{\tau}_{xy}^p + \lambda_1 \hat{\tau}_{xx}^p \frac{\partial \hat{u}}{\partial \hat{y}} + \alpha \frac{\lambda_1}{\hat{\eta}_p} \hat{\tau}_{xy}^p (\hat{\tau}_{xx}^p + \hat{\tau}_{yy}^p) - \hat{\eta}_p \frac{\partial \hat{u}}{\partial \hat{y}} = 0 \quad (5.8)$$

*Jaumann :*

If  $\hat{\tau}^p$  is the Jaumann stress tensor then, we have

$$\hat{\tau}_{xx}^p - \lambda_1 \hat{\tau}_{xy}^p \frac{\partial \hat{u}}{\partial \hat{y}} + \alpha \frac{\lambda_1}{\hat{\eta}_p} ((\hat{\tau}_{xx}^p)^2 + (\hat{\tau}_{xy}^p)^2) = 0 \quad (5.9)$$

$$\hat{\tau}_{yy}^p + \lambda_1 \hat{\tau}_{xy}^p \frac{\partial \hat{u}}{\partial \hat{y}} + \alpha \frac{\lambda_1}{\hat{\eta}_p} ((\hat{\tau}_{xy}^p)^2 + (\hat{\tau}_{yy}^p)^2) = 0 \quad (5.10)$$

$$\hat{\tau}_{xy}^p + \frac{1}{2} \lambda_1 (\hat{\tau}_{xx}^p - \hat{\tau}_{yy}^p) \frac{\partial \hat{u}}{\partial \hat{y}} + \alpha \frac{\lambda_1}{\hat{\eta}_p} \hat{\tau}_{xy}^p (\hat{\tau}_{xx}^p + \hat{\tau}_{yy}^p) - \hat{\eta}_p \frac{\partial \hat{u}}{\partial \hat{y}} = 0 \quad (5.11)$$

*Truesdell :*

Since the polymeric liquid is assumed incompressible, the velocity field is divergence free hence, for this the Truesdell rate constitutive equations for compressible matter become exactly same as those for upper convected case (i.e. (5.3) - (5.5)) for incompressible case.

## 5.2 Dimensionless form of the momentum and rate constitutive equations

When obtaining numerical solutions of the BVPs described by the mathematical model described by momentum and rate constitutive equations using methods of approximation, it is beneficial (and sometimes almost essential) to non-dimensionalize the GDEs in the mathematical model. For this purpose we use reference quantities. Let  $\rho_0$ ,  $u_0$ ,  $L_0$ ,  $\eta_0$ ,  $p_0$  and  $\tau_0$  be the reference density, velocity, length, viscosity, pressure and stress respectively. Then we define the following dimensionless quantities.

$$\rho = \hat{\rho}/\rho_0, u = \hat{u}/u_0, x = \hat{x}/L_0, y = \hat{y}/L_0, p = \hat{p}/p_0 \\ \tau^p = \hat{\tau}^p/\tau_0, \eta = \hat{\eta}/\eta_0, \eta_p = \hat{\eta}_p/\eta_0, \eta_s = \hat{\eta}_s/\eta_0, \hat{\eta} = \hat{\eta}_p + \hat{\eta}_s$$

We note that  $p_0$  and  $\tau_0$  are not independent ( $p_0 = \tau_0$  must hold). Generally we choose  $\tau_0 = \max((\tau_0)_{cke}, (\tau_0)_{cvs})$  [35, 36]. In which  $(\tau_0)_{cke}$  and  $(\tau_0)_{cvs}$  are reference stresses based on characteristic kinetic energy and characteristic viscous stress and are given by  $(\tau_0)_{cke} = \rho_0 u_0^2$  and  $(\tau_0)_{cvs} = \eta_0 u_0/L_0$ . If we define  $De = \lambda_1 u_0/L_0$ , Deborah number, then the dimensionless forms of the momentum and rate constitutive equations become:

*Momentum equations:*

In the absence of body forces we have

$$\left( \frac{p_0}{\rho_0 u_0^2} \right) \frac{\partial p}{\partial x} - \left( \frac{\tau_0}{\rho_0 u_0^2} \right) \left( \frac{\partial \tau_{xy}^p}{\partial y} + \left( \frac{\eta_0 u_0}{L_0 \tau_0} \right) \eta_s \frac{\partial^2 u}{\partial y^2} \right) = 0 \quad (5.12)$$

$$\left(\frac{p_0}{\rho_0 u_0^2}\right) \frac{\partial p}{\partial y} - \left(\frac{\tau_0}{\rho_0 u_0^2}\right) \frac{\partial \tau_{yy}^p}{\partial y} = 0 \quad (5.13)$$

*Rate constitutive equations:*

*Upper convected:*

$$\tau_{xx}^p - 2De \tau_{xy}^p \frac{\partial u}{\partial y} + \alpha \frac{De}{\eta_p} \left(\frac{L_0 \tau_0}{u_0 \eta_0}\right) ((\tau_{xx}^p)^2 + (\tau_{xy}^p)^2) = 0 \quad (5.14)$$

$$\tau_{yy}^p + \alpha \frac{De}{\eta_p} \left(\frac{L_0 \tau_0}{u_0 \eta_0}\right) ((\tau_{xy}^p)^2 + (\tau_{yy}^p)^2) = 0 \quad (5.15)$$

$$\tau_{xy}^p - De \tau_{yy}^p \frac{\partial u}{\partial y} + \alpha \frac{De}{\eta_p} \left(\frac{L_0 \tau_0}{u_0 \eta_0}\right) \tau_{xy}^p (\tau_{xx}^p + \tau_{yy}^p) - \left(\frac{u_0 \eta_0}{L_0 \tau_0}\right) \eta_p \frac{\partial u}{\partial y} = 0 \quad (5.16)$$

*Lower convected:*

$$\tau_{xx}^p + \alpha \frac{De}{\eta_p} \left(\frac{L_0 \tau_0}{u_0 \eta_0}\right) ((\tau_{xx}^p)^2 + (\tau_{xy}^p)^2) = 0 \quad (5.17)$$

$$\tau_{yy}^p + 2De \tau_{xy}^p \frac{\partial u}{\partial y} + \alpha \frac{De}{\eta_p} \left(\frac{L_0 \tau_0}{u_0 \eta_0}\right) ((\tau_{xy}^p)^2 + (\tau_{yy}^p)^2) = 0 \quad (5.18)$$

$$\tau_{xy}^p + De \tau_{xx}^p \frac{\partial u}{\partial y} + \alpha \frac{De}{\eta_p} \left(\frac{L_0 \tau_0}{u_0 \eta_0}\right) \tau_{xy}^p (\tau_{xx}^p + \tau_{yy}^p) - \left(\frac{u_0 \eta_0}{L_0 \tau_0}\right) \eta_p \frac{\partial u}{\partial y} = 0 \quad (5.19)$$

*Jaumann:*

$$\tau_{xx}^p - De \tau_{xy}^p \frac{\partial u}{\partial y} + \alpha \frac{De}{\eta_p} \left(\frac{L_0 \tau_0}{u_0 \eta_0}\right) ((\tau_{xx}^p)^2 + (\tau_{xy}^p)^2) = 0 \quad (5.20)$$

$$\tau_{yy}^p + De \tau_{xy}^p \frac{\partial u}{\partial y} + \alpha \frac{De}{\eta_p} \left(\frac{L_0 \tau_0}{u_0 \eta_0}\right) ((\tau_{xy}^p)^2 + (\tau_{yy}^p)^2) = 0 \quad (5.21)$$

$$\tau_{xy}^p + \frac{De}{2} (\tau_{xx}^p - \tau_{yy}^p) \frac{\partial u}{\partial y} + \alpha \frac{De}{\eta_p} \left(\frac{L_0 \tau_0}{u_0 \eta_0}\right) \tau_{xy}^p (\tau_{xx}^p + \tau_{yy}^p) - \left(\frac{u_0 \eta_0}{L_0 \tau_0}\right) \eta_p \frac{\partial u}{\partial y} = 0 \quad (5.22)$$

### 5.3 Numerical studies

In this section we present numerical studies for fully developed flow of a Giesekus fluid between parallel plates using all three rate constitutive equations. We choose PIB/C14 [37] fluid with the following properties.

$$\hat{\rho} = 800 \text{ kg/m}^3, \hat{\eta}_s = 0.002 \text{ Pa.s}, \hat{\eta}_p = 1.424 \text{ Pa.s}, \hat{\eta} = \hat{\eta}_s + \hat{\eta}_p = 1.426 \text{ Pa.s}, \alpha = 0.15$$

We also choose  $\eta_0 = \hat{\eta} = 1.426 \text{ Pa.s}$ , for which case we have  $\eta_s = \hat{\eta}_s/\eta_0 = 0.0015$  and  $\eta_p = \hat{\eta}_p/\eta_0 = 0.9985$  and the Reynolds number  $Re$  and Deborah number  $De$  are given by  $Re = (\rho_0 L_0/\eta_0)u_0 = 1.781206u_0$  and  $De = (\lambda_1/L_0)u_0 = 18.8976378u_0$  if we choose  $L_0 = 0.003175 = \hat{H}$ , half the distance between the parallel plates. The flow is pressure driven and is fully developed hence,  $\frac{\partial p}{\partial x}$  is known and must be specified for each study but  $\frac{\partial p}{\partial y}$  is related to  $\tau_{yy}^p$  through the  $y$ -momentum equation and is not known. We note that for the flow direction to be in the positive  $x$  direction,  $\frac{\partial p}{\partial x}$  must be negative. Progressively increasing magnitude of  $\frac{\partial p}{\partial x}$  result in progressively increasing flow rate and hence progressively increasing strain rates for which the behaviors of various rate constitutive equations can be investigated. An analytical solution of this BVP is not obtainable, hence we must resort to methods of approximation for obtaining numerical solutions. We use least squares finite element process in  $hpk$  framework.

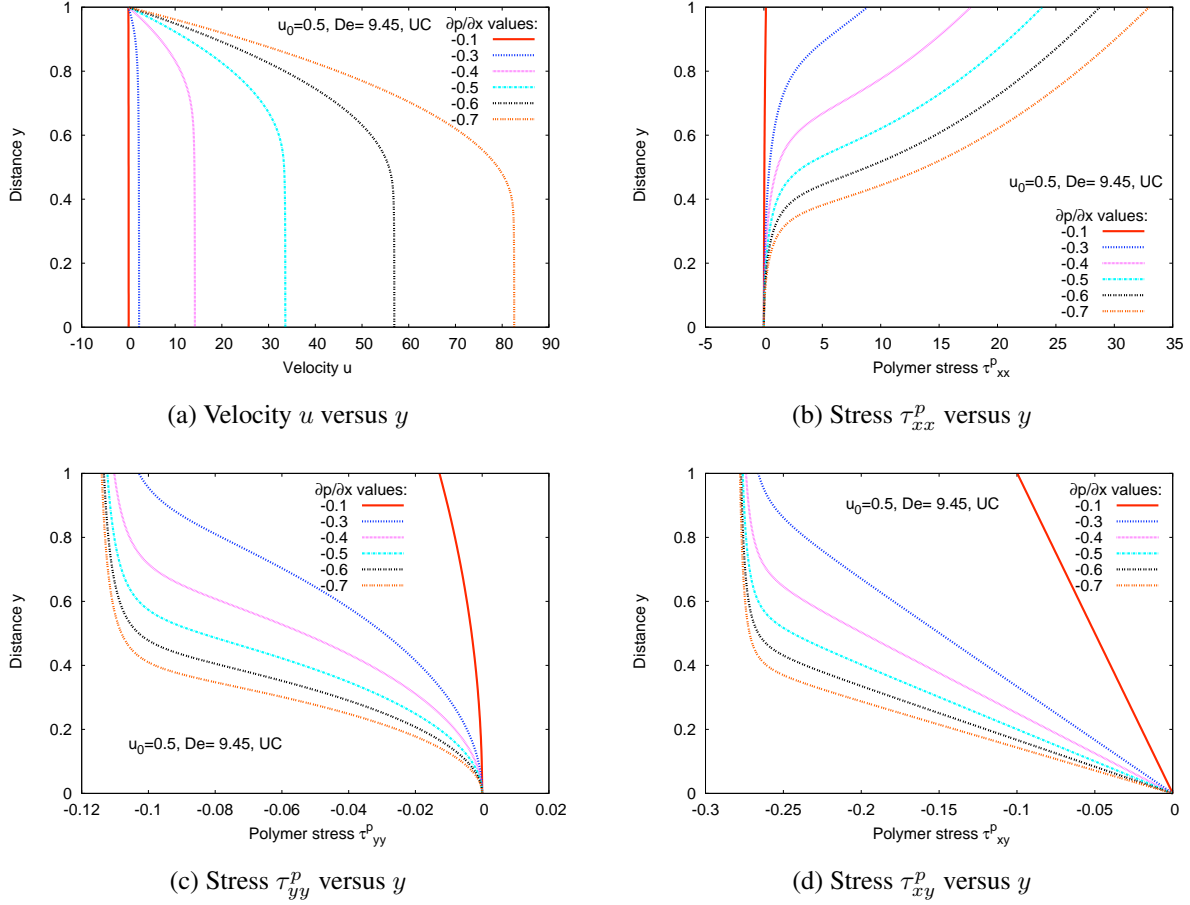


Figure 5.5: Velocity  $u$  and stress  $\tau^p$  in Giesekus fluids for upper convected rate equations

**Remarks:**

- (i) For this simple flow the solutions are expected to be smooth. Thus a relatively coarse mesh with minimally conforming  $k$  (the order of the approximation space) with progressively increasing  $p$ -levels are expected to yield converged solutions that satisfy GDEs accurately. If such solutions are in agreement with the flow physics then, these can be used as reference solutions. In the numerical studies we first establish that the upper convected (UC) rate constitutive equations indeed yield converged solutions independent of  $hp$  and  $k$  and that these satisfy GDEs accurately in the pointwise sense over the entire domain of the BVP and are in agreement with the flow physics.
- (ii) Converged solution obtained using lower convected (LC) and Jaumann (Jm) rate equations are then compared with those from the UC case to determine their validity: (a) for progressively increasing flow rate that correspond to the progressively increasing strain rates; (b) and for progressively increasing Deborah number ( $De$ ) for a fixed  $\frac{\partial p}{\partial x}$ .
- (iii) Surana et.al. [38] have shown that for this model problem a coarse uniform discretization of ten elements (half domain i.e.  $H$ ) with  $p$ -levels 5 – 11 for  $k = 2$  (solution of class  $C^1$  for  $u$ ,  $p$  and  $\tau^p$ ) produces converged solutions that satisfy GDEs quite well. Numerical studies reported for a twenty element uniform discretization confirm that indeed the ten element discretization has the same convergence rate but substantially lower  $I^e = \sum_e \sum_i (E_i^e, E_i^e)_{\bar{\Omega}^e}$ ;  $E_i^e$  being element residuals from the GDEs for a given DOFs due to the smoothness of the solution. Thus in all numerical studies we choose a ten element ( $p$ -version, 3-node elements) uniform discretization. We note that GDEs are a system of first order PDEs in  $p$  and  $\tau^p$  but the  $x$ -momentum equation contains second derivative of the velocity  $u$ . Thus minimally

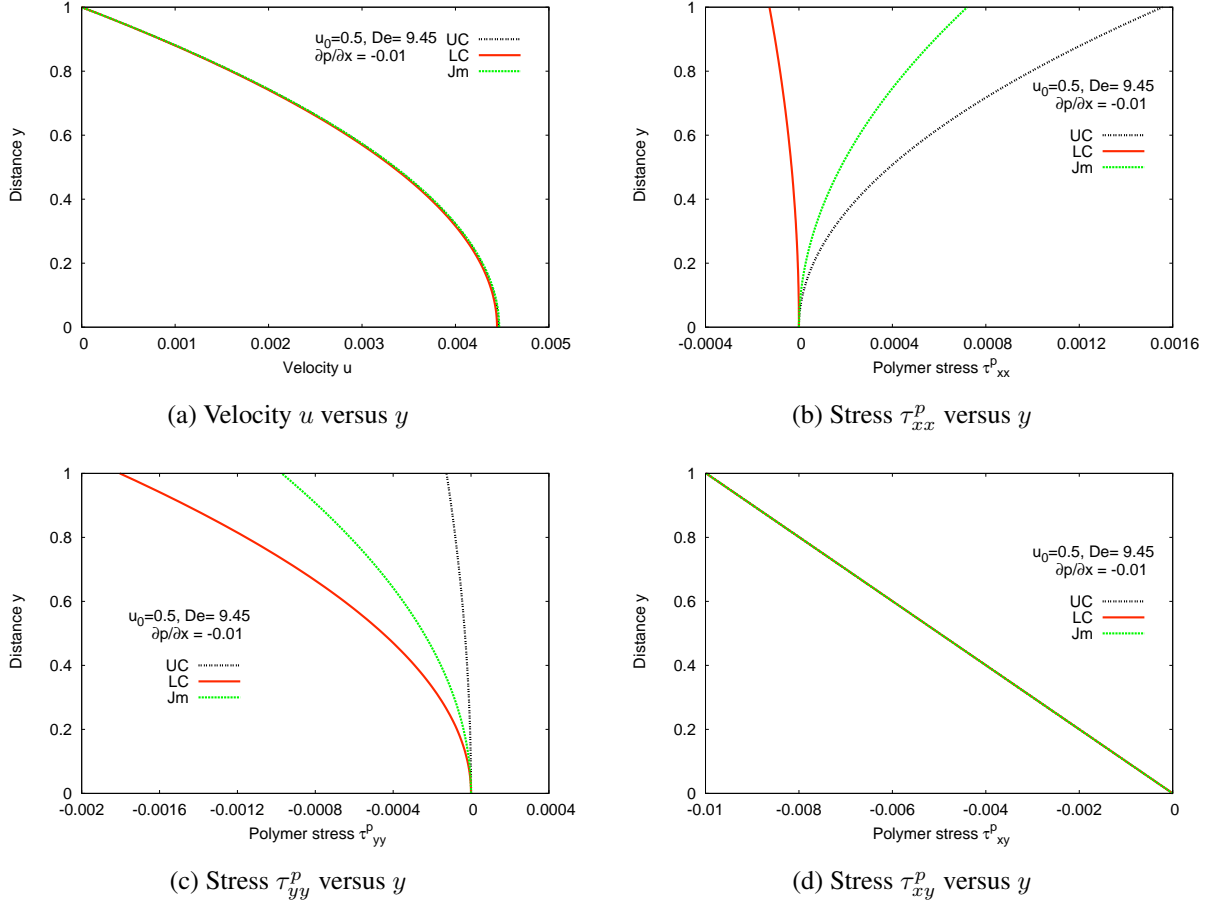


Figure 5.6: Velocity  $u$  and stress  $\tau^p$  for upper, lower convected and Jaumann rate equations at  $\frac{\partial p}{\partial x} = -0.01$

conforming  $k$  for  $p$  and  $\tau^p$  is two but  $k = 3$  is needed for the velocity  $u$  if the integrals are to be in the Riemann sense. Surana et.al. [38] have shown that choice of  $k = 2$  for velocity  $u$  suffices as well due to smoothness of the solution but for this choice the term corresponding to  $\frac{\partial^2 u}{\partial y^2}$  in the integrals are in Lebesgue sense. However, upon convergence the desired smoothness in the numerical solution is achieved [38]. In summary, for all numerical solution we choose a ten element uniform discretization with  $k = 2$  for  $u$ ,  $p$  and  $\tau^p$ . Based on reference [38]  $p$ -levels beyond 5 yield good accuracy of  $I$ . With  $p$ -levels of 11,  $I$  of the order of  $O(10^{-8})$  or lower is achieved indicating that the GDEs are satisfied accurately by the computed solutions.

(a) *Numerical studies for a fixed Deborah number with progressively increasing flow rates :*

In these studies we choose  $u_0 = 0.5$  which yield  $De = 9.45$  and  $Re = 0.89$  we also choose a ten element uniform mesh for  $\bar{\Omega} = H = 0 \leq y \leq 1$  using 3-node  $p$ -version elements with  $k = 2$  i.e. local approximations of class  $C^1(\bar{\Omega}^e)$  for  $u$ ,  $p$  as well as  $\tau^p$ . Based on reference [38] we choose  $p = 11$  for all dependent variables. Thus the local approximations for all dependent variables is of the same order and same degree. Figure 4 shows a schematic of the flow domain as well as boundary condition. Due to symmetry only the half of the domain (in  $y$  - direction) needs to be modeled. We consider upper half. The origin of the coordinate system  $xy$  is located at the center of the flow domain.  $x$  is the direction of the flow (left to right).

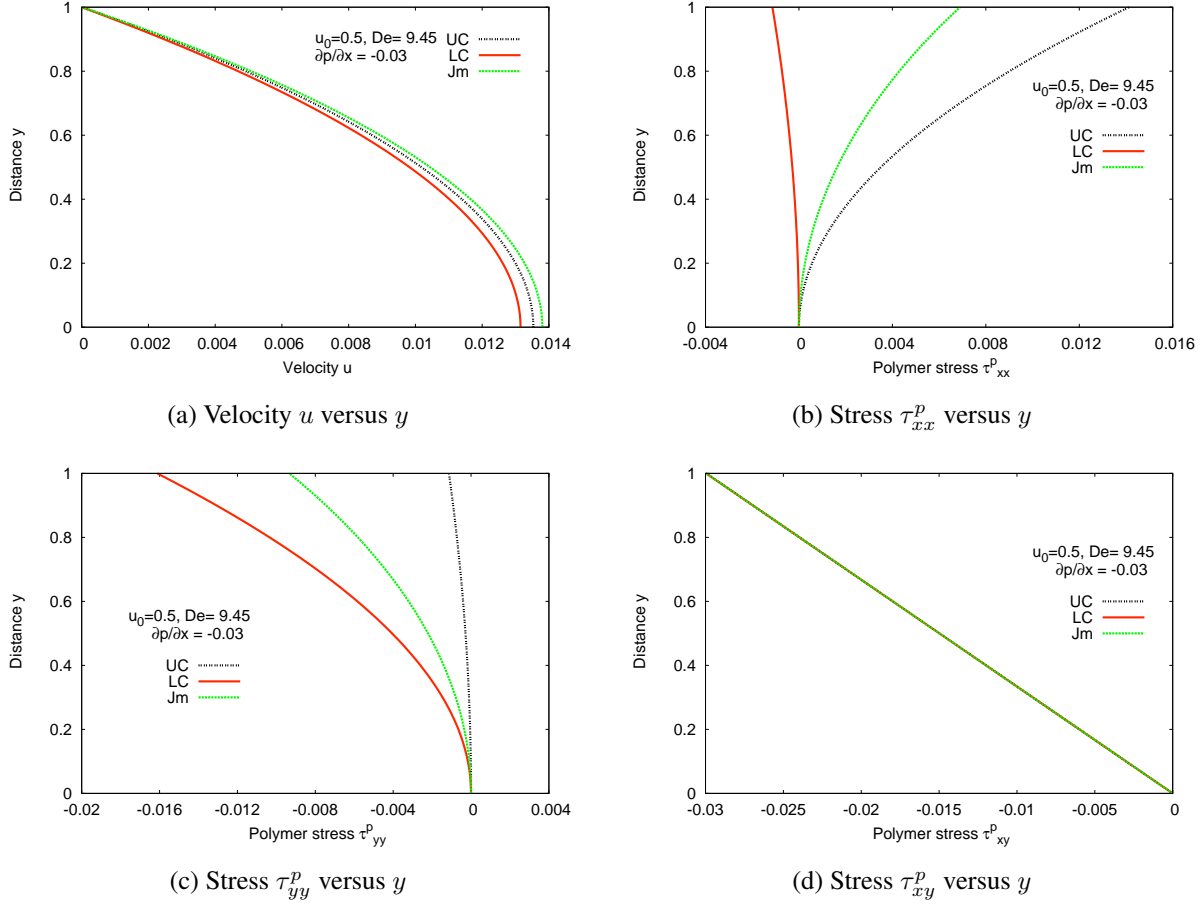


Figure 5.7: Velocity  $u$  and stress  $\tau^p$  for upper, lower convected and Jaumann rate equations at  $\frac{\partial p}{\partial x} = -0.03$

*Reference solution:*

First, we consider UC rate constitutive equations. We begin with  $\frac{\partial p}{\partial x} = -0.1$  and increment it by  $-0.1$  to obtain  $\frac{\partial p}{\partial x} = -0.1, -0.2, \dots$ . For each  $\frac{\partial p}{\partial x}$  we compute a numerical solution beginning with  $\frac{\partial p}{\partial x} = -0.1$  and by using a continuation procedure in  $\frac{\partial p}{\partial x}$ . That is, when computing a solution for  $\frac{\partial p}{\partial x} = -0.2$ , the converged solution at  $\frac{\partial p}{\partial x} = -0.1$  is used as initial solution or starting solution in Newton's linear method used for solving non-linear algebraic equations iteratively. This procedure is followed for each  $\frac{\partial p}{\partial x}$  value. For each  $\frac{\partial p}{\partial x}$  the least squares function  $I$  of the order of  $O(10^{-14})$  or lower is obtained indicating that the computed numerical solutions satisfy GDEs quite accurately. Newton's linear method converges in less than five iteration in all cases with good accuracy. The computed numerical results are shown in Figure 5 (a)-(d). From the velocity profiles in Figure 5(a), we note the progressively increasing maximum velocity at the center ( $y = 0$ ) for progressively increasing magnitude of  $\frac{\partial p}{\partial x}$ . As expected size of constant velocity core or plug at the center of the flow diminishes with increasing magnitude of  $\frac{\partial p}{\partial x}$ . Solutions for velocities are smooth, free of oscillations and conform to the flow physics. Plots of  $\tau^p_{xx}$ ,  $\tau^p_{yy}$  and  $\tau^p_{xy}$  versus distance  $y$  for different  $\frac{\partial p}{\partial x}$  values are shown in Figure 5 (b)-(d) are also smooth, oscillation free and conform to the flow physics (also see Surana et.al. [38]). Based on the values of  $I$  of  $O(10^{-14})$  and the results shown in Figure 5: (i) We can treat these solutions as reference solutions for evaluating the accuracy and legitimacy of the numerical solutions obtained by using LC and Jm rate constitutive equations. (ii) If there is a need to obtain a new reference solution for a different  $\frac{\partial p}{\partial x}$  (or  $De$ ) then we can use UC rate constitutive equations to do so. Keeping in mind that the low values of the least squares

functional  $I$  ( $I \leq O(10^{-14})$ ) and agreement of the solutions with the flow physics are two essential elements in judging whether a computed solution may serve as a reference solution. The numerical solution obtained using UC rate constitutive equations indeed satisfy these criteria.

*Comparisons of the solutions from UC, LC and Jm rate constitutive equations for a fixed  $De$  with increasing  $\frac{\partial p}{\partial x}$ :*

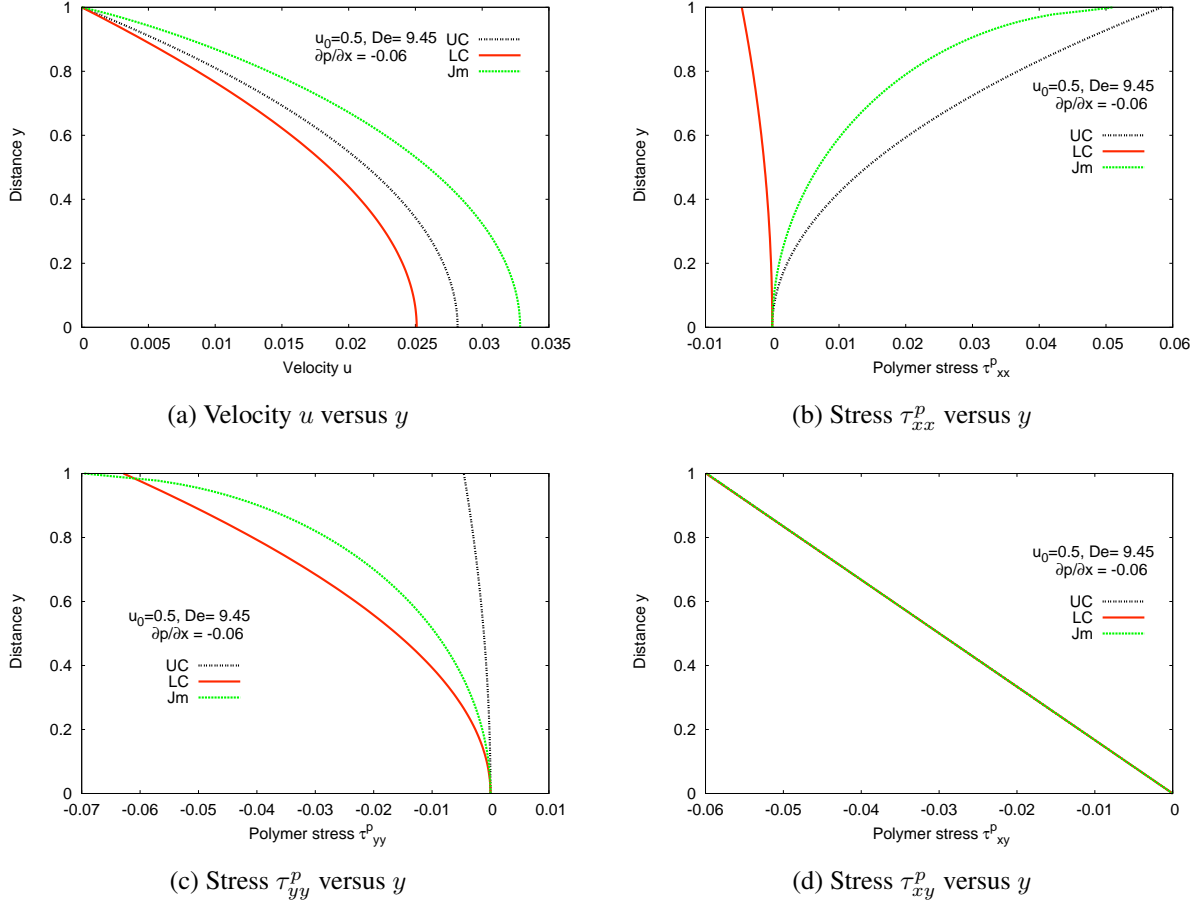


Figure 5.8: Velocity  $u$  and stress  $\tau^p$  for upper, lower convected and Jaumann rate equations at  $\frac{\partial p}{\partial x} = -0.06$

In this study we also choose  $u_0 = 0.5$  yielding  $De = 9.45$  and  $Re = 0.89$ .  $h, p$  and  $k$  remain the same as in the previous study i.e.  $h^e = H/10$ ,  $p = 11$  and  $k = 2$ . We choose  $\frac{\partial p}{\partial x} = -0.01$ . For this low value of  $\frac{\partial p}{\partial x}$ , we expect very low strain rates and hence UC, LC and Jm rate constitutive equations must show good agreement with each other. Next we consider  $\frac{\partial p}{\partial x} = -0.03$ , at this  $\frac{\partial p}{\partial x}$ , the strain rate(s) is much higher than that at  $\frac{\partial p}{\partial x} = -0.01$  and hence we shall observe some deviations of the results from LC and Jm when compared with UC. At  $\frac{\partial p}{\partial x} = -0.06$ , the strain rates are much higher and hence we shall observe the anomalous behaviors of LC and Jm rate constitutive equations and hence strong disagreement with UC. The computed numerical results for UC, LC and Jm rate constitutive equations for the three values of  $\frac{\partial p}{\partial x}$  are shown in Figure 6 - 8. In Figure 6(a) we note that the velocity profiles for UC, LC and Jm are all almost the same at  $\frac{\partial p}{\partial x} = -0.01$ . Hence for this case we expect the Jaumann stresses to be average of the UC and LC. This can be confirmed from Figures 6 (b)-(d). We clearly see that the polymer stresses from LC and Jm rate equations are significantly different compared to UC even for such low  $\frac{\partial p}{\partial x}$ . At  $\frac{\partial p}{\partial x} = -0.03$  (Figure 7 (a)-(d)) the velocity obtained from LC and Jm begin to deviate compared to

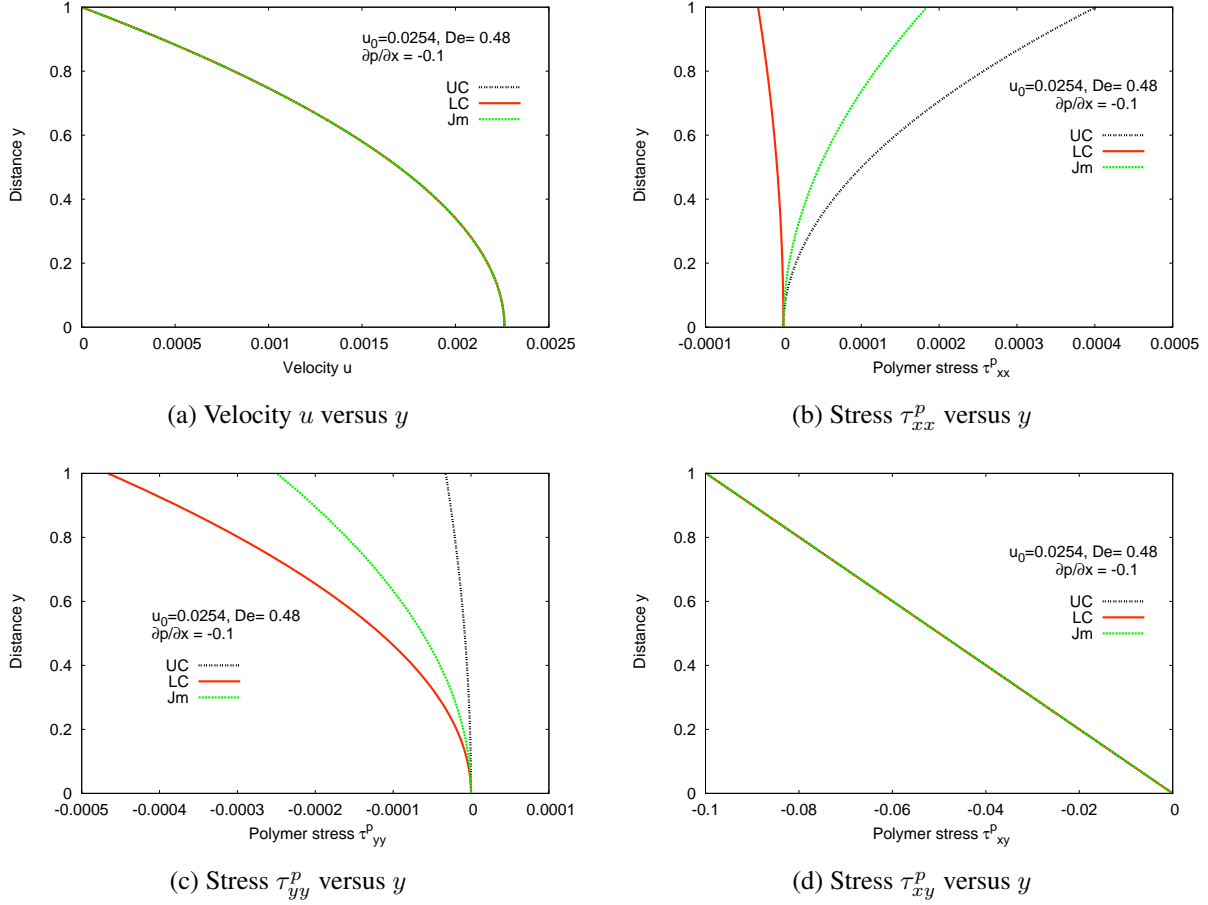


Figure 5.9: Velocity  $u$  and stress  $\tau^p$  for upper, lower convected and Jaumann rate equations at  $De = 0.48$

UC and hence the polymer stresses in Jm are no longer average of the polymer stress from UC and LC (except for  $\tau_{xy}^p$ ). This can be confirmed from the graphs shown in Figure 7 (b)-(d). At  $\frac{\partial p}{\partial x} = -0.06$  the velocities from LC and Jm are significantly different compared UC (Figure 8 (a)-(d)), keeping in mind that only UC results are physical as established earlier. The stresses  $\tau_{xx}^p$  and  $\tau_{yy}^p$  versus distance  $y$  in Figure 8 (b)-(c) conform: (i) Anomalous behaviors of LC and Jm rate constitutive equations; (ii)  $\tau_{xx}^p$  and  $\tau_{yy}^p$  from Jm are no longer average of the corresponding polymer stresses from UC and LC due to the differences in the velocity fields.  $\tau_{xy}^p$  continues to be linear (due to low value of  $\frac{\partial p}{\partial x}$  and low  $De$ ). For  $\frac{\partial p}{\partial x}$  beyond  $-0.06$ , Jm rate constitutive equation model experiences problems in the convergence of the Newton's method but LC continues to yield solutions that progressively deviate more and more from those obtained by UC. This study clearly demonstrates that infinitesimal strain assumption is essential for the validity of LC and Jm rate constitutive equations. The larger is the deviation from this assumption the more anomalous are the solutions of the BVPs incorporating the LC and Jm rate constitutive equations.

- (b) *Comparisons of the solutions from UC, LC and Jm rate constitutive equations for a fixed  $\frac{\partial p}{\partial x}$  with increasing  $De$ :*

In this study we choose a fixed value of  $\frac{\partial p}{\partial x} = -0.1$  and vary Deborah number by choosing  $u_0 = 0.0254, 0.254$  and  $0.385$  that yield  $De = 0.48, 4.8$  and  $7.28$  and Reynolds numbers of  $0.045, 0.452$  and  $0.686$ . We use uniform discretization of ten elements with  $p = 11$  and local approximation of class  $C^1$  for  $u, p$  and  $\tau^p$ . In all numerical studies reported here the least square functional values of  $O(10^{-14})$  or lower are achieved confirming that the computed solutions satisfy GDEs quite well. Just like in case of

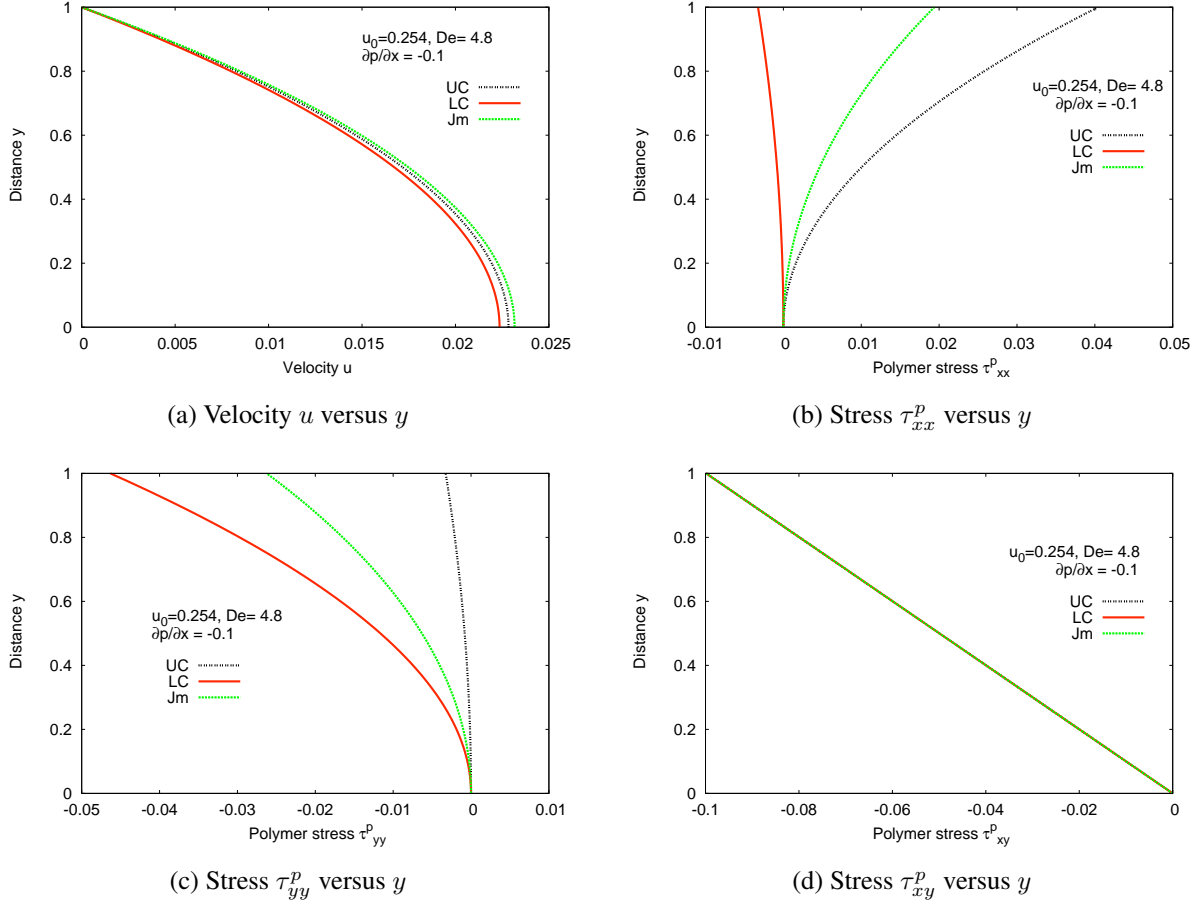


Figure 5.10: Velocity  $u$  and stress  $\tau^p$  for upper, lower convected and Jaumann rate equations at  $De = 4.8$

changing  $\frac{\partial p}{\partial x}$  in previous numerical study, here also we use continuation in Deborah number whenever needed i.e. using converged solutions at lower Deborah numbers as initial starting solution for higher Deborah numbers in the Newton's linear method for solving system of non-linear algebraic equations resulting from the assembly of the element equations.

Figure 9 (a)-(d) show graphs of  $u$ ,  $\tau_{xx}^p$ ,  $\tau_{yy}^p$  and  $\tau_{xy}^p$  versus  $y$  for  $De = 0.48$ . For this case, velocities  $u$  from UC, LC and Jm are in good agreement (due to very low strain rates) hence, polymer stresses from Jm are average of those from UC and LC as shown in Figure 9 (b)-(d). However, even for such low strain rates the  $\tau_{xx}^p$ ,  $\tau_{yy}^p$  from LC and Jm are significantly different compared to those from UC and hence are erroneous. Due to low strain rates for this  $De$ ,  $\tau_{xy}^p$  is almost linear for UC, LC and Jm rate constitutive equations (Figure 9(a)).

Figure 10 (a)-(d) show plots of  $u$ ,  $\tau_{xx}^p$ ,  $\tau_{yy}^p$  and  $\tau_{xy}^p$  versus  $y$  for  $De = 4.8$ . From Figure 9(a) we note that for this Deborah number the velocity fields from LC and Jm begin to deviate slightly compared to the velocity field from UC rate constitutive equations and as a consequence  $\tau_{xx}^p$  and  $\tau_{yy}^p$  from Jm are no longer average of those from UC and LC (Figures 9 (b)-(c)).  $\tau_{xy}^p$  is linear for all three rate constitutive equations (Figure 9(d)).

Plots of  $u$ ,  $\tau_{xx}^p$ ,  $\tau_{yy}^p$  and  $\tau_{xy}^p$  versus  $y$  for  $De = 7.28$  are shown in Figures 11 (a)-(d). For the Deborah number the velocity profiles from LC and Jm deviate significantly from the velocity profile for UC case. From Figures 11(b)-(c) we clearly observe that  $\tau_{xx}^p$  and  $\tau_{yy}^p$  from Jm are no longer average of those from UC and LC and are clearly anomalous when compared with UC rate constitutive equation.

Figures 12 (a)-(d) show plots of  $u$ ,  $\tau_{xx}^p$ ,  $\tau_{yy}^p$  and  $\tau_{xy}^p$  versus  $y$  for  $u_0 = 0.995$  yielding  $De = 18.8$  and

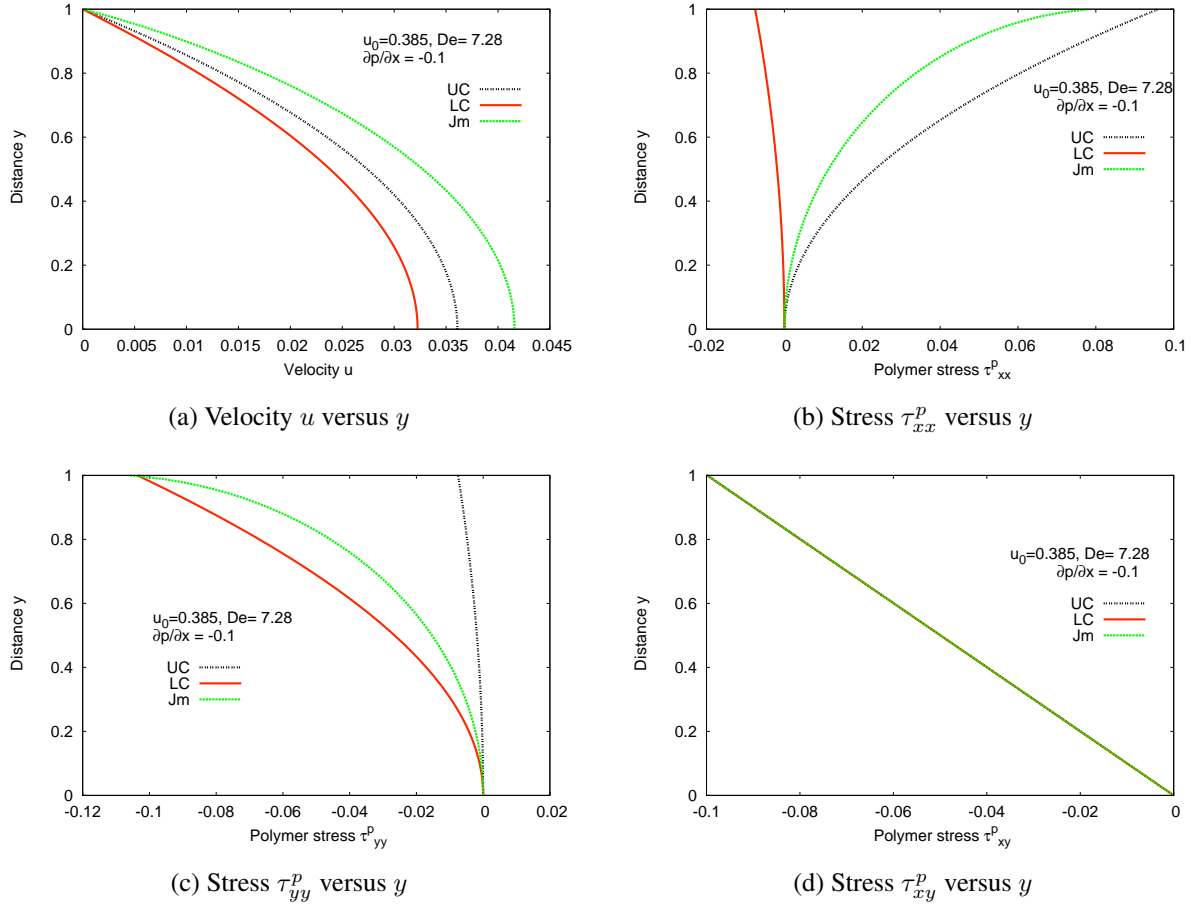


Figure 5.11: Velocity  $u$  and stress  $\tau^p$  for upper, lower convected and Jaumann rate equations at  $De = 7.28$

$Re = 1.77$  (keeping  $\frac{\partial p}{\partial x} = -0.1$ ). At this Deborah number Jm rate constitutive equations fail to yield results due to lack of convergence of the Newton's linear method. From Figures 12 (a)-(d) we note that LC rate constitutive equations yield numerical solutions that are completely spurious. The solution from the UC rate constitutive equations is smooth, free of oscillations and is in agreement with the physics and the solutions reported in reference [38]. At this higher  $De$ , we note that  $\tau_{xy}^p$  for UC rate constitutive equation is no longer linear (Figure 12(d)) whereas  $\tau_{xy}^p$  for LC continues to be linear.

(c) *Numerical studies for 2D developing flow between parallel plates:*

The numerical studies were also conducted for two dimensional developing flow between parallel plates for the same parameters as used for 1D fully developed flow presented here. These studies confirm that the fully developed flow results obtained from these (when converged) are in precise agreement with the solution presented here for UC, LC and Jm rate constitutive equations. The 2D developing flow studies presented by Surana et.al. [38] for UC rate constitutive equations also confirm this. The results of these studies are not presented here for the sake of brevity.

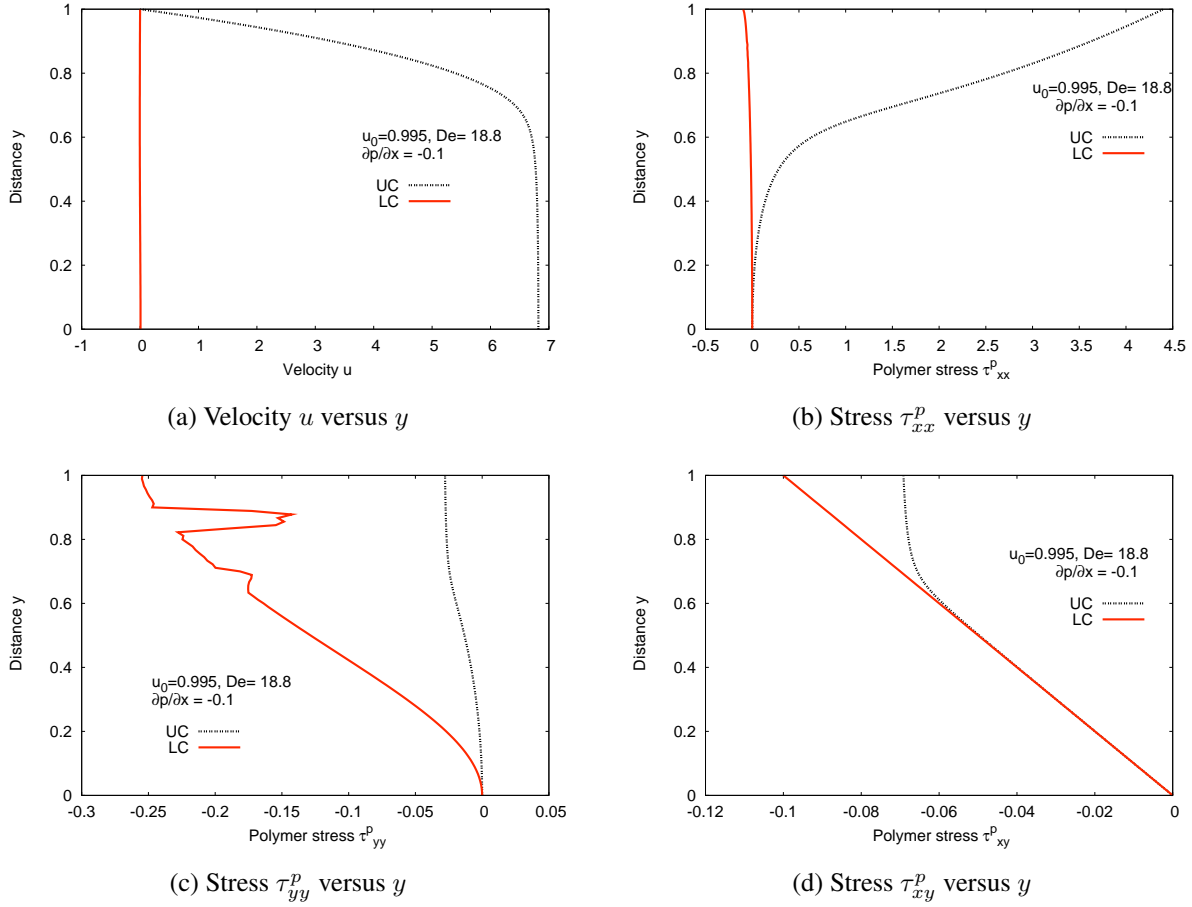


Figure 5.12: Velocity  $u$  and stress  $\tau^p$  for upper, lower convected and Jaumann rate equations at  $De = 18.8$

## 6 Summary and conclusions

The co-variant and contra-variant measures of the stresses and strains and their convected time derivatives in co- and contra-variant bases are presented. These derivations clearly demonstrate that only the contra-variant measures are based on true deformed tetrahedron in the current configuration. The co-variant measures of stresses and strains require a new tetrahedron configuration in the current configuration. It is shown that this tetrahedron configuration may be obtained by further deformation of the true deformed tetrahedron and hence is non-physical. Thus co-variant measures and their convected time derivatives are non-physical as well. When the deformation is small (infinitesimal), the true deformed tetrahedron used for contra-variant measures and the new distorted (or deformed) tetrahedron used in co-variant measures do not differ significantly and hence, in this case co- and contra-measures are almost the same. However, in case of finite deformation co- and contra-tetrahedron descriptions are significantly different. For finite deformation only contra-variant measures of stresses and strains and their convected time derivatives are physical.

Based on the co- and contra-variant stress and strain measures and their convected time derivatives, UC, LC, Jm and Truesdell rate constitutive equations commonly used in the published work are presented for solid deforming matter as well as dilute polymeric liquids and polymer melts. The upper convected rate constitutive equations are a contra-variant description, the lower convected rate constitutive equations are a co-variant description and Jaumann rate constitutive equations are an average of UC and LC when the velocity field in UC and LC cases are the same which is only possible for infinitesimal deformation. The Truesdell rate constitutive equations are also a contra-variant description with additional term  $div(\mathbf{v})\boldsymbol{\tau}$  to account for compressibility which is zero when the velocity field is divergence free as in case of incompressible matter (used in present

work). Since only the contra-variant descriptions are in agreement with the physics of deforming matter, only the UC rate constitutive equations are meaningful for finite deformation (noting that Truesdell rate constitutive equations are same as UC rate constitutive equation for divergence free velocity field).

Model problem studies are presented for fully developed flow of a Giesekus fluid between parallel plates. Since a theoretical solution is not available for this model problem, numerical solutions are obtained using least squares finite element methods in  $hpk$  framework. It is shown that the converged solutions (independent of  $h, p$  and  $k$ ) obtained by using UC rate constitutive equations (when the least squares functional  $I$  is of the order of  $O(10^{-14})$  or lower) can be used as reference solution. The numerical studies presented : (i) for a fixed Deborah number ( $De = 9.45$ ) with progressively increasing magnitude of  $\frac{\partial p}{\partial x}$ ; (ii) and those for a fixed  $\frac{\partial p}{\partial x} = -0.1$  with progressively increasing Deborah number show that the converged solutions from the UC rate constitutive equations always remain physical regardless of the strain rates while those from LC and Jm rate constitutive equations become progressively more anomalous with progressively increasing strain rates.

It is significant to note that a specific type of matter or a specific form of the rate equations is not the issue, the mayor issue is the choice of appropriate stress and strain measures and their convected time derivatives in the development of the rate constitutive equations. For example all rate constitutive equations regardless of the specific matter or their specific form that are based on, co-variant and Jaumann measures are bound to be non-physical for finite deformation as these measures and their convected time derivatives are non-physical for finite deformation. Likewise the use of contra-variant descriptions will incorporate the correct physics of the deforming matter and hence, is bound to yield more meaningful response of the deforming matter.

The issue of the lack of thermodynamics basis for the rate constitutive equation is not addressed in this chapter. This work only addresses the legitimacy of the rate constitutive equations based on chosen measures of stresses and strains and their convected time derivatives and the meritoriousness of one rate constitutive equation over the others in terms of its ability to produce physically meaningful response for progressively increasing deformation leading to finite deformation.

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## Chapter 6

# Summary, Conclusions and Future Work

The research work in this report represents the development of rate constitutive theories for compressible and incompressible matter in co-variant and contra-variant bases using axioms and principles of continuum mechanics. In all developments we consider the deforming matter to be homogeneous and isotropic, and thus the constitutive theory at a material point is valid for all material points in the deforming matter. The rate constitutive theories are required in mathematical models of deforming matter derived using conservation laws in the Eulerian description in which material particle displacements and strain measures are not easily obtainable. Therefore, a constitutive theory expressing the stress tensor (and heat vector) as a function of strain measures is not possible. Instead, we must consider time derivatives of the strain measures as well as stress measures in the development of the constitutive theory.

The co-variant basis in the current configuration identifying deformed material lines and the reciprocal contra-variant basis are natural choices for the development of the rate constitutive theory. In these two convected coordinate systems we define the co-variant and contra-variant Cauchy stress tensors, both being symmetric tensors of rank two. We consider Green's and Almansi strain tensors as measures of finite strain in co-variant and contra-variant bases and derive their convected time derivatives up to order  $n$  in the respective convected coordinate systems. These definitions are the same regardless of whether the matter is compressible or incompressible. These convected time derivatives of the strain measures constitute fundamental kinematic tensors. We also derive the convected time derivatives of up to order  $m$  of the co-variant and contra-variant Cauchy stress tensors in the respective bases for compressible as well as incompressible matter. These convected time derivatives of the stress and strain measures are objective and hence are admissible in the development of the constitutive theory.

Since conservation of mass, balance of momenta, and conservation of energy are independent of the constitution of the matter, the second law of thermodynamics (fourth conservation law), i.e., entropy inequality, known as the Clausius-Duhem inequality, must form the basis for the development of the rate constitutive theory. It is shown that in the Eulerian description, the conditions resulting from the second law of thermodynamics establish the Cauchy stress tensor, heat vector, and Helmholtz free energy density as dependent variables in the constitutive theory but do not provide a mechanism for the development of the rate constitutive theory for the Cauchy stress tensor (in the co-variant and contra-variant bases). This is resolved by decomposing the Cauchy stress tensor into equilibrium stress tensor and deviatoric Cauchy stress tensor. The conditions resulting from the entropy inequality are used to establish the equilibrium stress for compressible matter as thermodynamic pressure, function of density and temperature in the current configuration. In the case of incompressible matter, incompressibility constraint in conjunction with the conditions resulting from the entropy inequality are used to establish the equilibrium stress as mechanical pressure, function of temperature in the current configuration. Thus, the constitutive relations for the equilibrium stress are completely established for compressible as well as incompressible matter. Therefore, the constitutive theory reduces to the determination of the deviatoric Cauchy stress tensor (in contra- and co-variant bases) in addition to the heat vector and Helmholtz free energy density. We remark that the conditions resulting from the entropy inequality can also be used to establish the constitutive relation for the heat vector resulting in the well known Fourier heat conduction law. However, it is shown that a more complete and realistic constitutive theory for the heat vector is possible using the alternate approach presented in this work. At this stage we note that the conditions resulting from the entropy inequality

require the dissipation due to the deviatoric Cauchy stress to be positive but they provide no mechanism for the development of the constitutive theory for it.

By examining the constitute theory for solid matter in Lagrangian description derived strictly based on the conditions resulting from the entropy inequality we observe that the stress tensor is expressed as a linear combination of the generators of the argument strain tensor. This suggest that in the development of the rate constitutive theory we can consider the following approach: (i) Identify argument tensors of the dependent variables in the constitutive theory: deviatoric Cauchy stress tensor, heat vector and Helmholtz free energy density. (ii) Determine the combined generators using the argument tensors of rank two and one. In the case of the deviatoric Cauchy stress tensor (symmetric tensor of rank two), the combined generators must be symmetric tensors of rank two whereas in the case of the heat vector (a tensor of rank one), the combined generators of its argument tensors (of rank two and one) must be of rank one. (iii) Express the deviatoric Cauchy stress tensor and the heat vector as a linear combination of the combined generators of their argument tensors. The coefficients in the linear combinations are functions of the combined invariants of the argument tensors, density  $\bar{\rho}$  and temperature  $\bar{\theta}$  (in the current configuration). (iv) The coefficients in the linear combinations are determined by considering their Taylor's series expansions about the reference configuration and by limiting the expansions to linear terms in the combined invariants and temperature  $\bar{\theta}$ . This approach constitutes the basic methodology presented in this research for the development of rate constitutive theories in co-variant and contra-variant bases.

The rate constitutive theory for ordered thermofluids has been presented. It is shown that for compressible ordered thermofluids: (i) in contra-variant basis, the argument tensors of deviatoric stress  $[_d\bar{\sigma}^{(0)}]$  and heat vector  $\bar{\mathbf{q}}^{(0)}$  are  $\bar{\rho}$ ,  $\bar{\theta}$ ,  $\bar{\mathbf{g}}$  and  $[\gamma^{(j)}]$ ;  $j = 1, 2, \dots, n$  the convected time derivatives of orders  $1, 2, \dots, n$  in the contra-variant basis and for  $\bar{\Phi}$ , the argument tensors are  $\bar{\rho}$  and  $\bar{\theta}$ . (ii) in co-variant basis, the argument tensors of the deviatoric stress  $[_d\bar{\sigma}_{(0)}]$  and heat vector  $\bar{\mathbf{q}}_{(0)}$  are  $\bar{\rho}$ ,  $\bar{\theta}$ ,  $\bar{\mathbf{g}}$  and  $[\gamma_{(j)}]$ ;  $j = 1, 2, \dots, n$  the convected time derivatives of orders  $1, 2, \dots, n$  in the co-variant basis and for  $\bar{\Phi}$ , the argument tensors are  $\bar{\rho}$  and  $\bar{\theta}$ . For incompressible ordered thermofluids, density  $\bar{\rho}$  in the current configuration is the same as in the reference configuration and hence it is no longer an argument of the dependent variables in the constitutive theory. Other arguments remain the same as for the compressible case. The theory of generators and invariants is utilized to derive the general form of the constitutive theory for an  $n^{th}$  order 'ordered thermofluid' (both compressible and incompressible) in contra-variant and co-variant bases. In this theory both the deviatoric stress and the heat vectors are expressed as a linear combination of the combined generators of the argument tensors. The coefficients in this linear combination are functions of the combined invariants of the argument tensors in addition to  $\bar{\rho}$  and  $\bar{\theta}$  (in case of compressible fluids) or  $\bar{\theta}$  (in case of incompressible fluids). The coefficients are determined by using their Taylor series expansion about the reference configuration and retaining only up to linear terms in the combined invariants and temperature. Explicit details are presented for second order 'ordered thermofluids'. The general form of the constitutive equations are specialized and detailed derivations are presented for thermoviscous generalized Newtonian and Newtonian fluids (both compressible and incompressible). For such fluids, only the first convected time derivative of the strain tensor (Green or Almansi depending upon co-variant or contra-variant basis) remains as argument tensor for the deviatoric stress (in addition to density and temperature). The heat vector does not contain the first convected time derivative of the strain tensor as an argument. A significant point to note is that all constitutive equations for ordered thermofluids in contra-variant or co-variant bases are in fact rate constitutive equations. In the case of constitutive equations in the contra-variant basis, we express the convected time derivative of order zero of the contra-variant Cauchy stress tensor  $[_d\bar{\sigma}^{(0)}]$  in terms of the convected time derivatives of various orders of the Almansi strain tensor in the contra-variant basis. Likewise, for the constitutive equations in the co-variant basis, we express the convected time derivative of order zero of the co-variant Cauchy stress tensor  $[_d\bar{\sigma}_{(0)}]$  in terms of the convected time derivatives of various orders of the Green's strain tensor in the co-variant basis. Thus, the constitutive equation for generalized Newtonian and Newtonian fluid are indeed rate constitutive equations. The distinction between co- and contra-variant measures disappears for such fluids due to the fact that the convected time derivative of order one of the Green's strain is the same as the convected time derivative of order one of the Almansi strain with the additional restriction of infinitesimal deformation. We also note that, based on the work of Surana et al., when the deformation is finite, only the constitutive equations derived using contra-variant basis remain valid. As the magnitude of the deformation increases, the constitutive equations in co-variant basis and others become progressively more spurious.

In the case of the rate constitutive theory for ordered thermoelastic solids, it is shown that for compressible thermoelastic solids, in contra-variant basis, the argument tensors of the first convected time derivative of the deviatoric Cauchy stress  $[\bar{d}\bar{\sigma}^{(0)}]$ , i.e.,  $[\bar{d}\bar{\sigma}^{(1)}]$  and the heat vector  $\bar{\mathbf{q}}^{(0)}$  are  $\bar{\rho}$ ,  $\bar{\theta}$ ,  $\bar{\mathbf{g}}$  and  $[\gamma^{(j)}]$ ;  $j = 1, 2, \dots, n$  the convected time derivatives of orders  $1, 2, \dots, n$  in the contra-variant basis and for  $\bar{\Phi}$ , the argument tensors are  $\bar{\rho}$  and  $\bar{\theta}$ . In co-variant basis, the argument tensors of the first convected time derivative of the deviatoric stress  $[\bar{d}\bar{\sigma}_{(0)}]$  i.e.,  $[\bar{d}\bar{\sigma}_{(1)}]$  and the heat vector  $\bar{\mathbf{q}}_{(0)}$  are  $\bar{\rho}$ ,  $\bar{\theta}$ ,  $\bar{\mathbf{g}}$  and  $[\gamma_{(j)}]$ ;  $j = 1, 2, \dots, n$  the convected time derivatives of orders  $1, 2, \dots, n$  in the co-variant basis and for  $\bar{\Phi}$ , the argument tensors are  $\bar{\rho}$  and  $\bar{\theta}$ . For incompressible ordered thermoelastic solids, density  $\bar{\rho}$  in the current configuration is the same as in the reference configuration and hence it is no longer an argument of the dependent variables in the constitutive theory. Other arguments remain the same as for the compressible case. The theory of generators and invariants is utilized to derive the general form of the constitutive equations for an  $n^{th}$  order ‘ordered thermoelastic solid’ (both compressible and incompressible) in contra-variant and co-variant bases. In this theory both the first convected time derivative of the deviatoric stress and the heat vector are expressed as a linear combination of the combined generators of the argument tensors. The coefficients in this linear combination are functions of the combined invariants of the argument tensors in addition to  $\bar{\rho}$  and  $\bar{\theta}$  (in case of compressible solids) or  $\bar{\theta}$  (in case of incompressible solids). The coefficients in the linear combinations are determined by using their Taylor’s series expansion about the reference configuration and retaining only up to linear terms in the combined invariants and temperature. Explicit details are presented for second order ‘ordered thermoelastic solids’. The general form of the constitutive equations are specialized and detailed derivations are presented for thermoelastic solids of order two and one as well as hypo-thermoelastic solids. We note that the rate constitutive equations derived here for an ordered thermoelastic solid of order ‘ $n$ ’ express the first convected time derivative of the stress tensor as a function of density  $\bar{\rho}$ , temperature  $\bar{\theta}$ , temperature gradient  $\bar{\mathbf{g}}$  and the convected time derivatives of the conjugate strain tensor of up to order ‘ $n$ ’ in a chosen basis i.e., contra- or co-variant. The contra-variant basis yields upper convected rate constitutive equations whereas co-variant basis gives lower convected rate constitutive equations. Surana et al. have shown that in the case of finite deformation, only upper convected rate constitutive equations are in conformity with the physics of deformation. Definitions of  $[\bar{d}\bar{\sigma}^{(1)}]$  and  $[\bar{d}\bar{\sigma}_{(1)}]$  differ when the deformation is finite. Furthermore, the definition of  $[\bar{d}\bar{\sigma}^{(1)}]$  is different for compressible and incompressible matter. Same is the case for  $[\bar{d}\bar{\sigma}_{(1)}]$ . In the case of compressible matter  $[\bar{d}\bar{\sigma}^{(1)}]$  is the Truesdell rate. Definitions of  $[\bar{d}\bar{\sigma}^{(1)}]$  and  $[\bar{d}\bar{\sigma}_{(1)}]$  differ when the deformation is finite. Furthermore, the definition of  $[\bar{d}\bar{\sigma}^{(1)}]$  is different for compressible and incompressible matter. Same is the case for  $[\bar{d}\bar{\sigma}_{(1)}]$ . In the case of compressible matter  $[\bar{d}\bar{\sigma}^{(1)}]$  is the Truesdell rate. For ordered thermoelastic solids of order greater than or equal to two, the argument tensors  $[\gamma^{(1)}]$  and  $[\gamma_{(1)}]$  are the same but the argument tensors  $[\gamma^{(j)}]$ ;  $j = 2, 3, \dots$  and  $[\gamma_{(j)}]$ ;  $j = 2, 3, \dots$  differ. The rate constitutive equations in contra-variant and co-variant bases are not the same if we deviate from the infinitesimal deformation assumption. The first order rate constitutive equations ( $n = 1$ ) are simplified to obtain constitutive equations for what is commonly known as hypo-elastic material, restricted to infinitesimal deformation. To be more precise, in this case, second and higher order terms in the components of the first convected time derivatives of the strain tensor are assumed negligible. Thus, use of such constitutive relations for finite deformation is not justified.

The rate constitutive theory for ordered thermoviscoelastic fluids considers convected time derivatives of up to order  $m$  of the deviatoric stress tensor and convected time derivatives of up to order ‘ $n$ ’ of the strain tensor in the chosen basis. The convected time derivative of order  $m$  of the deviatoric stress tensor, the heat vector  $\bar{\mathbf{q}}$  and Helmholtz free energy density  $\bar{\Phi}$  are considered as dependent variables in the development of the rate constitutive theory. Based on the principle of equipresence, the argument tensors of these dependent variables are considered to be  $[\gamma^{(j)}]$ ;  $j = 1, 2, \dots, n$ ,  $[\bar{d}\bar{\sigma}^{(k)}]$ ;  $k = 0, 1, \dots, m-1$ , density  $\bar{\rho}$ , temperature  $\bar{\theta}$  and temperature gradient  $\bar{\mathbf{g}}$  in the contra-variant basis. In the case of co-variant basis,  $[\gamma^{(j)}]$  and  $[\bar{d}\bar{\sigma}^{(k)}]$  are replaced by  $[\gamma_{(j)}]$  and  $[\bar{d}\bar{\sigma}_{(k)}]$  while the other arguments remain the same. These rate constitutive equations define an ordered thermoviscoelastic fluid of orders  $(m, n)$ . In this approach  $[\bar{d}\bar{\sigma}^{(m)}]$  and  $\bar{\mathbf{q}}$  or  $[\bar{d}\bar{\sigma}_{(m)}]$  and  $\bar{\mathbf{q}}$  are expressed as a linear combination of the combined generators of the argument tensors keeping in mind that  $[\bar{d}\bar{\sigma}^{(m)}]$  and  $[\bar{d}\bar{\sigma}_{(m)}]$  are symmetric tensors of rank two where as  $\bar{\mathbf{q}}$  is a tensor of rank one. Hence, the combined generators used in the linear combinations for  $[\bar{d}\bar{\sigma}^{(m)}]$  or  $[\bar{d}\bar{\sigma}_{(m)}]$  must also be symmetric tensors of rank two. Whereas the combined generators used to define  $\bar{\mathbf{q}}$  must be tensors of rank one. Additionally we must also adhere to minimal basis in these linear combinations. The coefficients in the linear combinations are functions of density  $\bar{\rho}$ , temperature  $\bar{\theta}$  and the combined invariants of the argument tensors of rank one and two and are determined

by considering their Taylor series expansion about the reference configuration and limiting the expansion up to linear terms in the combined invariants and  $\bar{\theta}$ . The general theory of rate constitutive equations is specialized for  $m = 1$  and  $n = 1$ , i.e., thermoviscoelastic fluids of order one in stress and strain rates. In this case  $[_d\bar{\sigma}^{(1)}]$  or  $[_d\bar{\sigma}_{(1)}]$  contain  $[_d\bar{\sigma}^{(0)}]$ ,  $[\gamma^{(1)}]$ ,  $\bar{\rho}$ ,  $\bar{\theta}$ ,  $\bar{\mathbf{g}}$  or  $[_d\bar{\sigma}_{(0)}]$ ,  $[\gamma_{(1)}]$ ,  $\bar{\rho}$ ,  $\bar{\theta}$ ,  $\bar{\mathbf{g}}$  as argument tensors in contra- and co-variant bases. The same argument tensors also hold for the heat vector  $\bar{\mathbf{q}}$ . The general theory is also specialized for  $m = 1$  and  $n = 2$ , i.e., thermoviscoelastic fluids of order one in stress rate but of order two in strain rate. In this case  $[_d\bar{\sigma}^{(1)}]$  or  $[_d\bar{\sigma}_{(1)}]$  contain  $[_d\bar{\sigma}^{(0)}]$ ,  $[\gamma^{(1)}]$ ,  $[\gamma^{(2)}]$ ,  $\bar{\rho}$ ,  $\bar{\theta}$ ,  $\bar{\mathbf{g}}$  or  $[_d\bar{\sigma}_{(0)}]$ ,  $[\gamma_{(1)}]$ ,  $[\gamma_{(2)}]$ ,  $\bar{\rho}$ ,  $\bar{\theta}$ ,  $\bar{\mathbf{g}}$  as argument tensors in contra- and co-variant bases. The same argument tensors also hold for the heat vector  $\bar{\mathbf{q}}$ . It is shown that Maxwell constitutive model and Giesekus constitutive model are a subset of ordered thermoviscoelastic fluids (incompressible) of orders  $m = 1$  and  $n = 1$ . Derivations presented in the report demonstrate many assumptions needed for the general case of  $m = 1$ ,  $n = 1$  to derive these constitutive models. Maxwell model is a linear viscoelastic model whereas Giesekus constitutive model is a non-linear constitutive model. It is also shown that Oldroyd-B constitutive model is a subset of the rate constitutive equations of orders  $m = 1$  and  $n = 2$ . The derivation presented in the report demonstrates many assumptions that must be employed for the general case of  $m = 1$  and  $n = 2$  to derive Oldroyd-B constitutive model. This constitutive model is referred to as quasi-linear constitutive model. The Maxwell, Oldroyd-B and Giesekus constitutive models as used in polymer science have been derived using kinetic theory. The reference to the Maxwell model based on continuum mechanics can be found in some published work. However, the derivations of Oldroyd-B and Giesekus constitutive models based on principles and axioms of continuum mechanics as presented in this report are the first appearance of this work in the published literature to our knowledge. The derivations of Maxwell, Oldroyd-B and Giesekus constitutive models presented here are fundamental in understanding the assumptions employed in their derivations which eventually limit their range of applications. For example, all three constitutive models are only valid for non-finite deformation for which the distinction between co- and contra-variant bases is irrelevant. Giesekus model is superior in terms of more realistic  $[_d\bar{\sigma}^{(0)}]$  or  $[_d\bar{\sigma}_{(0)}]$  due to inclusion of  $[_d\bar{\sigma}^{(0)}]^2$  or  $[_d\bar{\sigma}_{(0)}]^2$ .

The contra-variant basis yields upper convected ordered rate constitutive equations. Likewise, the co-variant basis yields lower convected ordered rate constitutive equations. Surana et al. have shown that only contra-variant basis is in accordance with the physics of deforming matter when the deformation is finite. As the deformation deviates from the infinitesimal assumption, the rate constitutive equations based on co-variant basis and others (such as Jaumann rate equations) become progressively spurious with progressively increasing deformation. Theoretical work as well as numerical studies are presented (using Giesekus constitutive model) to demonstrate this aspect.

Based on the theory of generators and invariants, the constitutive equation for the heat vector for an ordered matter is much more complex, even for thermofluids of order one due to the dependence of the heat vector on the combined generators of  $[\gamma^{(1)}]$ ,  $\bar{\mathbf{g}}$  or  $[\gamma_{(1)}]$ ,  $\bar{\mathbf{g}}$ , compared to Fourier heat conduction law which requires that the heat vector not be dependent on  $[\gamma^{(1)}]$  or  $[\gamma_{(1)}]$ . The constitutive equation for the heat vector based on the combined generators of  $[\gamma^{(1)}]$ ,  $\bar{\mathbf{g}}$  or  $[\gamma_{(1)}]$ ,  $\bar{\mathbf{g}}$  is perhaps more realistic for fluids as it accounts for velocity gradients. However, their use will require experimental determination of additional constants or coefficients. In all three rate theories, consistent derivation of the constitutive theory for the heat vector has been presented by utilizing the same argument tensors as in the case of the deviatoric Cauchy stress tensor.

The rate constitutive theories presented in this report provide the most general infrastructure for the development of constitutive equations for compressible as well as incompressible ordered thermofluids, thermoelastic solids and the thermoviscoelastic fluids in co-variant and contra-variant bases. These constitutive theories are essential when the mathematical models are derived using Eulerian descriptions. It is shown that regardless of the matter, the constitutive equations in Eulerian descriptions are always rate constitutive equations. The ordered theories provide means of incorporating the desired physics in the development of the constitutive relations. It has been shown that the constitutive relations for Newtonian fluids, generalized Newtonian fluids, hypo-elastic solids, Maxwell fluids, Oldroyd-B fluids and Giesekus fluids that are commonly used in the literature are all subsets of the general rate theories presented here. The derivations of these specific constitutive models from the general rate theories reveal many assumptions employed which in term limit the physics that can be described by the resulting constitutive models. It is shown that most rate constitutive equations used presently are only valid for non-finite deformation in which case the distinction between co- and contra-variant descriptions disappears. Even though Green's strain and Almansi strain tensors are measures of finite deformation, their first convected time derivatives in both co- and contra-variant bases are not. Thus the constitutive

theories that only utilize the first convected time derivative of the strain tensor (such as Newtonian fluids, generalized Newtonian fluids, hypo-elastic solids, Maxwell model, Giesekus model) are all limited to non-finite deformation. The choice of dependent variables in the rate constitutive theories is based on the second law of thermodynamics and not ad-hoc as the choice of polymer stress as dependent variable in the Giesekus constitutive model used currently.

The work presented here suggests several areas of future research. Some key areas are listed below:

- (1) Development of rate constitutive theories for finite deformation based on the concept of ordered theories.
- (2) Many investigations to compare the theories suggested by the rate theories with those used currently. Giesekus model is an example.
- (3) We note that the coefficients or constants in the rate constitutive theory resulting after Taylor series expansions are with respect to the reference configuration. In deforming matter experiencing finite deformation in which subsequent deformed configurations may be significantly different than the reference configuration, the use of these coefficients or constants needs justification. Perhaps a new strategy is needed for their redetermination based on progressively deformed configurations of the matter.
- (4) The Fourier heat conduction law used universally for all deforming matters was originally proposed by Fourier for solid matter. The new constitutive theories presented here for the heat vector suggest constitutive relations that incorporate the influence of the velocity field and its interaction with temperature gradients. This is perhaps more realistic for liquids and gases but requires determination of additional coefficients or constants experimentally.
- (5) Development of constitutive theories for materials with memory including phase transition encompassing shape memory materials.
- (6) A unified constitutive theory of plasticity in Lagrangian and Eulerian descriptions based on the second law of thermodynamics that incorporates flow theories as well as strain space theories. This suggested research is parallel as well as in contrast to the Endochronic theory of Valanis. In contrast to the works of Valanis, the proposed theory shows no intrinsic time scale as advocated by Valanis. This work requires development of finite deformation theories in conjunction with the constitutive theories for elasto-plastic deformation based on the second law of thermodynamics. This work is crucial in applications such as blast, impact, penetration etc.

This short list represents just a few obvious areas of research suggested by the work presented in this report. Closer examinations of the derivations of currently used constitutive models using general rate constitutive theories presented in this work suggest many better alternatives for more realistic physics in the constitutive theories but at the expense of the determination of additional coefficients or constants by designing prudent experiments. We hope to contribute in these areas of research that are much neglected but are of paramount significance in yielding mathematical models that would incorporate the desired physics and would produce meaningful and realistic results for varied physics encountered in practical applications.